STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 173736

TO: Ben Sackey **Location: rem-5b31/5c18** **Art Unit: 1626** **December 9, 2005** **Case Serial Number: 10/673988**	**From: P. Sheppard** **Location: Remsen Building** **Phone: (571) 272-2529** **sheppard@uspto.gov**

Search Notes

FOR OFFICIAL USE ONLY 173736 ACCESS DB # _____
PLEASE PRINT CLEARLY

Paula

Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: BEN SACKEY Examiner #: 73489 Date: 12/8/05
Art Unit: 1626 Phone Number: 2-0704 Serial Number: 10/673,988
Location (Bldg/Room#): REM 5B31 (Mailbox #): C18 Results Format Preferred (circle): ~~PAPER~~ DISK

****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: Method of producing alkoxymalononitriles

Inventors (please provide full names): Bartek et al

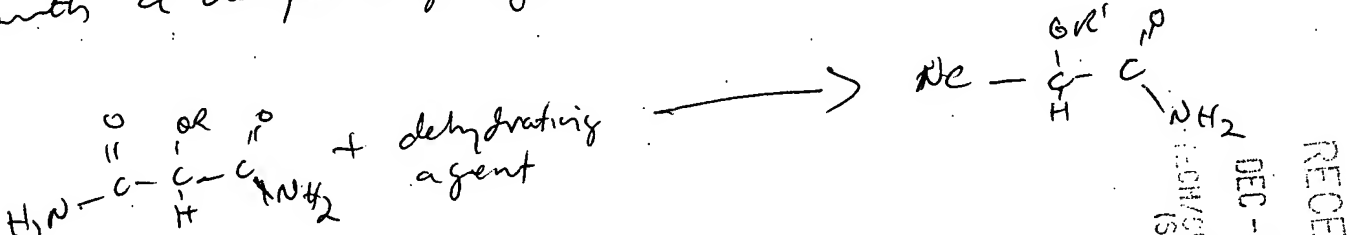
Earliest Priority Date: 5/04/00.

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

A process for preparing 2-cyano-2-alkoxyacetamides of formula (III): Comprising reacting alkoxymalonamides of formula (II) with a dehydrating agent:



eg of dehydrating agents

trifluoroacetic ~~acid~~ anhydride
dibutyltin oxide, phosphorus oxychloride
phosphorus trichloride

```
=> d his ful

     (FILE 'HCAPLUS' ENTERED AT 16:19:52 ON 09 DEC 2005)

     FILE 'REGISTRY' ENTERED AT 16:58:12 ON 09 DEC 2005
L1              STR
L3           31 SEA SSS FUL L1
L6              STR
L8          158 SEA SSS FUL L6
L9           49 SEA ABB=ON  PLU=ON  TRIFLUOROACETIC ANHYDRIDE?/CN OR DIBUTYLTIN
                 OXIDE?/CN OR PHOSPHORUS OXYCHLORIDE?/CN OR PHOSPHORUS
                TRICHLORIDE?/CN OR PHOSPHORUS PENTACHLORIDE?/CN
L11         643 SEA ABB=ON  PLU=ON  ALUMINUM CHLORIDE?/CN

     FILE 'HCAPLUS' ENTERED AT 17:06:09 ON 09 DEC 2005
L12           8 SEA ABB=ON  PLU=ON  L3
                D STAT QUE
                D IBIB ABS HITSTR L12 1-8
L13          70 SEA ABB=ON  PLU=ON  L8
L14       25437 SEA ABB=ON  PLU=ON  L9 OR TRIFLUOROACETIC(W)ANHYDRIDE OR
                DIBUTYLTIN(W) OXIDE OR PHOSPHORUS(W)(OXYCHLORIDE? OR TRICHLORID
                E OR PENTACHLORIDE?)
L15       73122 SEA ABB=ON  PLU=ON  L11 OR ALUMINUM (W)CHLORIDE OR ALCL3
L16      389244 SEA ABB=ON  PLU=ON  ("DEHYDRATION AGENTS"/CV OR "DEHYDRATION
                REACTION (L) AGENTS"/CV OR "DRYING AGENTS"/CV) OR DEHYDRAT? OR
                DRYING
L17       30094 SEA ABB=ON  PLU=ON  ("LEWIS ACIDS"/CV OR "CARBONYLS (L) LEWIS
                ACID COMPLEXES"/CV OR "CHARGE TRANSFER COMPLEXES"/CV OR
                ELECTROPHILES/CV OR "LEWIS ACIDITY"/CV OR "LEWIS BASES"/CV) OR
                LEWIS(W)ACID
L20           4 SEA ABB=ON  PLU=ON  (L8 AND (L16 OR L14 OR L17 OR L15)) NOT
                L12
L21        1744 SEA ABB=ON  PLU=ON  CYANO(L)?ACETAMIDE?
L22           1 SEA ABB=ON  PLU=ON  (L21 AND L13) NOT L12
L23           5 SEA ABB=ON  PLU=ON  L20 OR L22
                D STAT QUE
                D IBIB ABS HITSTR L23 1-5
L24          62 SEA ABB=ON  PLU=ON  ("BARTEK J"/AU OR "BARTEK J P"/AU) OR
                "BARTEK JOHANNES"/AU
L25         222 SEA ABB=ON  PLU=ON  ("FUCHS R"/AU OR "FUCHS R A"/AU OR "FUCHS
                R E M"/AU OR "FUCHS R F"/AU OR "FUCHS R J"/AU OR "FUCHS R
                K"/AU OR "FUCHS R L"/AU OR "FUCHS R M"/AU OR "FUCHS R P"/AU OR
                "FUCHS R P P"/AU OR "FUCHS R R"/AU OR "FUCHS R WAYNE"/AU) OR
                "FUCHS RUDOLF"/AU
L26          15 SEA ABB=ON  PLU=ON  "HILDBRAND STEFAN"/AU
L27          14 SEA ABB=ON  PLU=ON  L26 NOT (L12 OR L20)
                D STAT QUE L27 NOS
                D IBIB ABS L27 1-14
L29           0 SEA ABB=ON  PLU=ON  ((L24 OR L25) AND L13) NOT (L12 OR L20 OR
                L27)
L30        5603 SEA ABB=ON  PLU=ON  (L16 OR L14) AND (L17 OR L15)

     FILE 'REGISTRY' ENTERED AT 17:17:32 ON 09 DEC 2005
L31        1285 SEA ABB=ON  PLU=ON  MALONAMIDE?

     FILE 'HCAPLUS' ENTERED AT 17:17:57 ON 09 DEC 2005
L32        3721 SEA ABB=ON  PLU=ON  L31 OR ?MALOMAMIDE?
L33           8 SEA ABB=ON  PLU=ON  L32 AND L30
L34           7 SEA ABB=ON  PLU=ON  L33 NOT (L12 OR L20 OR L27)
                D STAT QUE L29
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              D STAT QUE L34
              D IBIB ABS HITSTR L34 1-7

     FILE 'CASREACT' ENTERED AT 17:26:39 ON 09 DEC 2005
L35           0 SEA SSS SAM L1 (     0 REACTIONS)
L36           2 SEA SSS FUL L1 (    35 REACTIONS)
              D STAT QUE
              D IBIB ABS RXS 1-2


     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:     8 DEC 2005  HIGHEST RN 869627-02-1
     DICTIONARY FILE UPDATES:    8 DEC 2005  HIGHEST RN 869627-02-1

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

     TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

       Please note that search-term pricing does apply when
       conducting SmartSELECT searches.

     ************************************************************
     *                                                          *
     * The CA roles and document type information have been removed from *
     * the IDE default display format and the ED field has been added,   *
     * effective March 20, 2005.  A new display format, IDERL, is now    *
     * available and contains the CA role and document type information. *
     *                                                          *
     ************************************************************

     Structure search iteration limits have been increased.  See HELP SLIMITS
     for details.

     REGISTRY includes numerically searchable data for experimental and
     predicted properties as well as tags indicating availability of
     experimental property data in the original document.  For information
     on property searching in REGISTRY, refer to:

     http://www.cas.org/ONLINE/UG/regprops.html

     FILE HCAPLUS

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     FILE COVERS 1907 - 9 Dec 2005  VOL 143 ISS 25
     FILE LAST UPDATED: 8 Dec 2005  (20051208/ED)

     New CAS Information Use Policies, enter HELP USAGETERMS for details.
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This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE CASREACT

FILE CONTENT:1840 - 4 Dec 2005 VOL 143 ISS 23

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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*
* CASREACT now has more than 10 million reactions *
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

```
=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 17:06:09 ON 09 DEC 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 9 Dec 2005  VOL 143 ISS 25
FILE LAST UPDATED: 8 Dec 2005  (20051208/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=>
=>

=> d stat que
L1                STR
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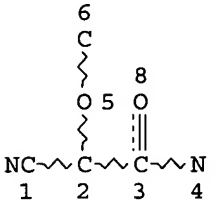


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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   7

STEREO ATTRIBUTES: NONE
L3            31 SEA FILE=REGISTRY SSS FUL L1
L12            8 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3


=>
=>

=> d ibib abs hitstr l12 1-8

L12  ANSWER 1 OF 8  HCAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2004:804106  HCAPLUS
DOCUMENT NUMBER:          142:23494
```

TITLE: Three-Component Condensation Leading to β-Amino Acid Diamides: Convergent Assembly of β-Peptide Analogues

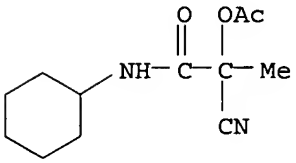
AUTHOR(S): Oaksmith, Jennifer M.; Peters, Ulf; Ganem, Bruce
CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Baker Laboratory, Cornell University, Ithaca, NY, 14853-1301, USA

SOURCE: Journal of the American Chemical Society (2004), 126(42), 13606-13607
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:23494

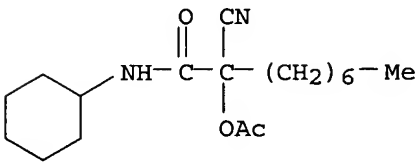
AB A Passerini condensation of acyl cyanides, carboxylic acids, and isonitriles has been developed that affords efficient access to functionalized diamides as well as β-peptides of α-hydroxy-β-amino acids. Such compds.. are protease-resistant and form stable helical and sheet structures when incorporated into larger peptides (no data given). N-Protected α-amino acids and isocyanoesters derived from α-amino acids participate in the condensation, leading to α/β peptides embodying the heterogeneous α/β/α backbone motif.

IT **799778-66-8P 799778-69-1P 799778-85-1P 799778-93-1P 799779-04-7P 799779-09-2P 799779-13-8P 799779-16-1P 799779-25-2P 799779-30-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (acyloxy)(cyano)carboxamides via via Passerini condensation of acyl cyanides, carboxylic acids, and isonitriles)

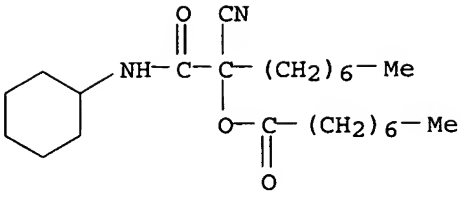
RN 799778-66-8 HCAPLUS
CN Propanamide, 2-(acetyloxy)-2-cyano-N-cyclohexyl- (9CI) (CA INDEX NAME)



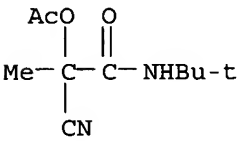
RN 799778-69-1 HCAPLUS
CN Nonanamide, 2-(acetyloxy)-2-cyano-N-cyclohexyl- (9CI) (CA INDEX NAME)



RN 799778-85-1 HCAPLUS
CN Octanoic acid, 1-cyano-1-[(cyclohexylamino)carbonyl]octyl ester (9CI) (CA INDEX NAME)

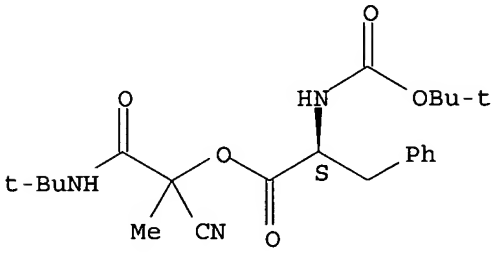


RN 799778-93-1 HCAPLUS
CN Propanamide, 2-(acetyloxy)-2-cyano-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

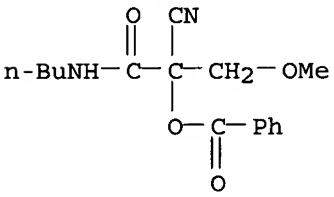


RN 799779-04-7 HCAPLUS
CN L-Phenylalanine, N-[(1,1-dimethylethoxy)carbonyl]-, 1-cyano-2-[(1,1-dimethylethyl)amino]-1-methyl-2-oxoethyl ester (9CI) (CA INDEX NAME)

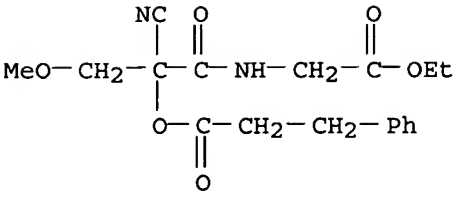
Absolute stereochemistry.



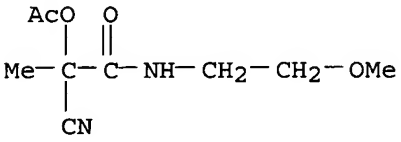
RN 799779-09-2 HCAPLUS
CN Propanamide, 2-(benzoyloxy)-N-butyl-2-cyano-3-methoxy- (9CI) (CA INDEX NAME)



RN 799779-13-8 HCAPLUS
CN Benzenepropanoic acid, 1-cyano-2-[(2-ethoxy-2-oxoethyl)amino]-1-(methoxymethyl)-2-oxoethyl ester (9CI) (CA INDEX NAME)

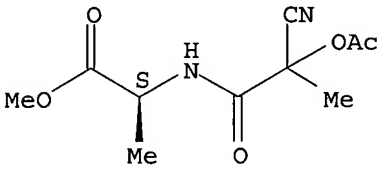


RN 799779-16-1 HCAPLUS
CN Propanamide, 2-(acetyloxy)-2-cyano-N-(2-methoxyethyl)- (9CI) (CA INDEX NAME)



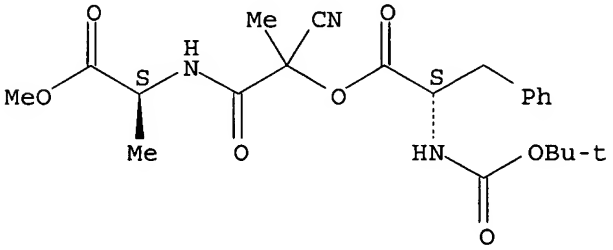
RN 799779-25-2 HCAPLUS
CN L-Alanine, N-[2-(acetyloxy)-2-cyano-1-oxopropyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 799779-30-9 HCAPLUS
CN 3,8-Dioxa-5,11-diazatridecan-13-oic acid, 9-cyano-2,2,9,12-tetramethyl-4,7,10-trioxo-6-(phenylmethyl)-, methyl ester, (6S,12S)- (9CI) (CA INDEX NAME)

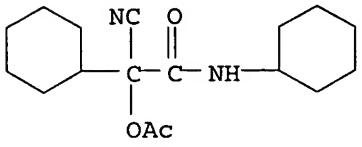
Absolute stereochemistry.



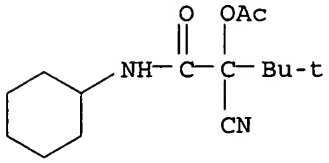
IT **799778-72-6P 799778-75-9P 799778-78-2P**
799778-81-7P 799778-83-9P 799778-88-4P
799778-90-8P 799778-98-6P 799779-01-4P
799779-07-0P 799779-11-6P 799779-19-4P
799779-22-9P 799779-28-5P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of (acyloxy)(cyano)carboxamides via via Passerini condensation of acyl cyanides, carboxylic acids, and isonitriles)

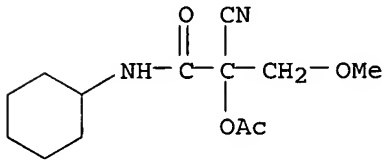
RN 799778-72-6 HCAPLUS
CN Cyclohexaneacetamide, α-(acetyloxy)-α-cyano-N-cyclohexyl- (9CI) (CA INDEX NAME)



RN 799778-75-9 HCAPLUS
CN Butanamide, 2-(acetyloxy)-2-cyano-N-cyclohexyl-3,3-dimethyl- (9CI) (CA INDEX NAME)

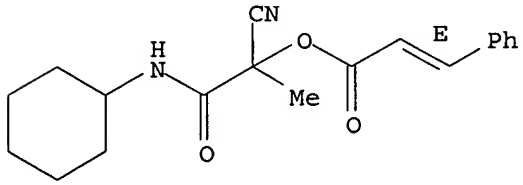


RN 799778-78-2 HCAPLUS
CN Propanamide, 2-(acetyloxy)-2-cyano-N-cyclohexyl-3-methoxy- (9CI) (CA INDEX NAME)

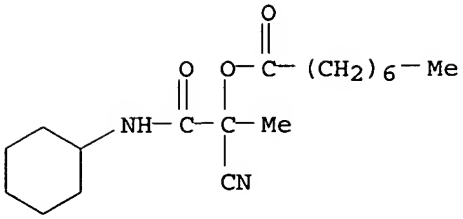


RN 799778-81-7 HCAPLUS
CN 2-Propenoic acid, 3-phenyl-, 1-cyano-2-(cyclohexylamino)-1-methyl-2-oxoethyl ester, (2E)- (9CI) (CA INDEX NAME)

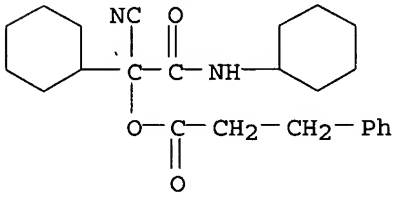
Double bond geometry as shown.



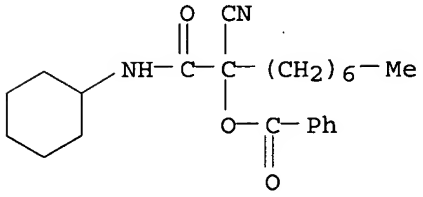
RN 799778-83-9 HCAPLUS
CN Octanoic acid, 1-cyano-2-(cyclohexylamino)-1-methyl-2-oxoethyl ester (9CI) (CA INDEX NAME)



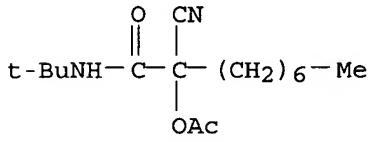
RN 799778-88-4 HCAPLUS
CN Benzenepropanoic acid, 1-cyano-1-cyclohexyl-2-(cyclohexylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



RN 799778-90-8 HCAPLUS
CN Nonanamide, 2-(benzoyloxy)-2-cyano-N-cyclohexyl- (9CI) (CA INDEX NAME)

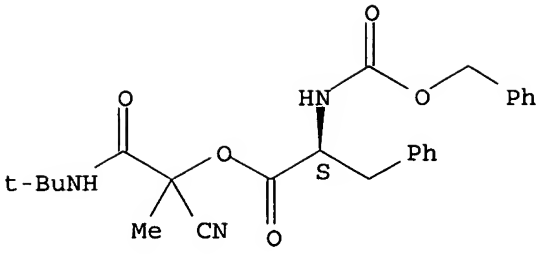


RN 799778-98-6 HCAPLUS
CN Nonanamide, 2-(acetyloxy)-2-cyano-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

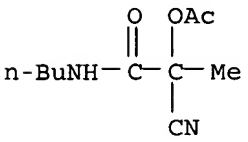


RN 799779-01-4 HCAPLUS
CN L-Phenylalanine, N-[(phenylmethoxy)carbonyl]-, 1-cyano-2-[(1,1-dimethylethyl)amino]-1-methyl-2-oxoethyl ester (9CI) (CA INDEX NAME)

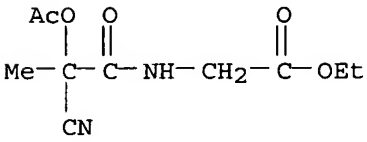
Absolute stereochemistry.



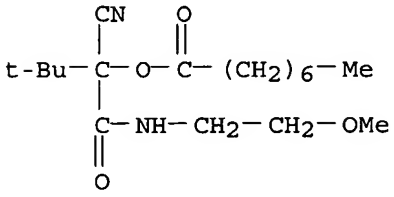
RN 799779-07-0 HCAPLUS
CN Propanamide, 2-(acetyloxy)-N-butyl-2-cyano- (9CI) (CA INDEX NAME)



RN 799779-11-6 HCAPLUS
CN Glycine, N-[2-(acetyloxy)-2-cyano-1-oxopropyl]-, ethyl ester (9CI) (CA INDEX NAME)

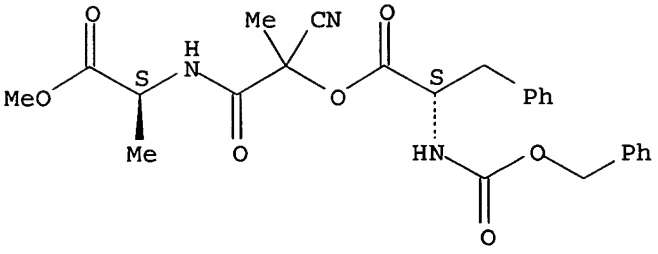


RN 799779-19-4 HCAPLUS
CN Octanoic acid, 1-cyano-1-[[(2-methoxyethyl)amino]carbonyl]-2,2-dimethylpropyl ester (9CI) (CA INDEX NAME)



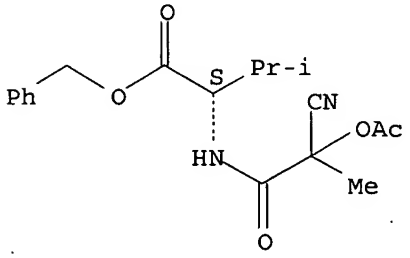
RN 799779-22-9 HCAPLUS
CN 2,7-Dioxa-4,10-diazadodecan-12-oic acid, 8-cyano-8,11-dimethyl-3,6,9-trioxo-1-phenyl-5-(phenylmethyl)-, methyl ester, (5S,11S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 799779-28-5 HCAPLUS
CN L-Valine, N-[2-(acetyloxy)-2-cyano-1-oxopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:749510 HCAPLUS
DOCUMENT NUMBER: 138:32334
TITLE: Reactions of Mn(III) quadridentate Schiff base compounds with TCNQ anion to form unusual TCNQ derivatives by alcoholysis
AUTHOR(S): Miyasaka, Hitoshi; Sugimoto, Kunihisa; Sugiura, Ken-Ichi; Ishii, Tomohiko; Yamashita, Masahiro
CORPORATE SOURCE: Department of Chemistry, Graduate School of Science, Tokyo Metropolitan University, Tokyo, 192-0397, Japan
SOURCE: Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (2002), 379, 197-204
CODEN: MCLCE9; ISSN: 1058-725X
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The reactions of Mn(III) quadridentate Schiff base compds., [Mn(saltmen)(H2O)]ClO4 (1; saltmen2- = N,N'-(1,1,2,2-tetramethylethylene)bis(salicylideneiminato)) and [Mn(naphtmen)(H2O)]ClO4 (2; naphtmen2- = N,N'-(1,1,2,2-tetramethylethylene)bis(naphthylideneiminato)), with LiTCNQ gave three types of compds. depending on reaction conditions: [Mn(saltmen)(H2O)](TCNQ) (3), [Mn(saltmen)(MeOH)(TCNQ-OMe)] (4, TCNQ-OMe- = p-(α,α-dicyano-α-methoxytolyl)dicyanomethanide), and [Mn(naphtmen)(MeOH)(TCNQA-OMe)] (5, TCNQA-OMe- = p-(α-cyano-α-methoxy-α-methylamidotolyl)dicyanomethanide). Compds. 3·MeOH and 5 were characterized by x-ray crystallog. Compds. 3 and 4 were prepared under

anaerobic and aerobic conditions, resp., in MeOH/H2O. Compound 5 was synthesized under aerobic conditions analogous to 4. For 4 and 5, unusual addition reactions on the anionic TCNQ mol. occurred to form (TCNQ-OMe)- for 4 and (TCNQA-OMe)- for 5. Ferromagnetic and antiferromagnetic interactions in the prepared compds. were investigated.

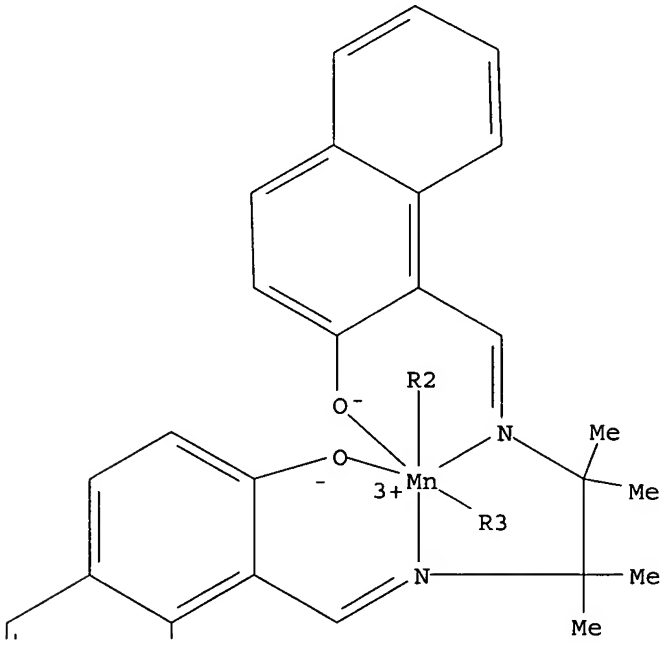
IT **478158-45-1P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal structure, and magnetic properties of)

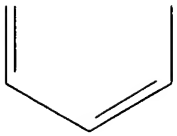
RN 478158-45-1 HCAPLUS

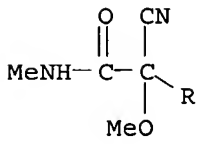
CN Manganese, [α-cyano-4-[1-cyano-2-(imino-κN)ethenyl]-α-methoxy-N-methylbenzeneacetamidato](methanol)[[1,1'-[(1,1,2,2-tetramethyl-1,2-ethanediyl)bis[(nitrilo-κN)methylidyne]]bis[2-naphthalenolato-κO]](2-)]-, (OC-6-34)- (9CI) (CA INDEX NAME)

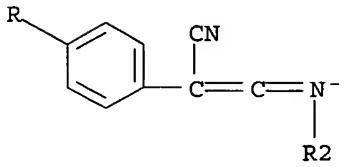
PAGE 1-A



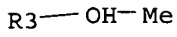
PAGE 2-A







PAGE 3-A



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:597946 HCAPLUS
DOCUMENT NUMBER: 135:152562
TITLE: Dehydration method for producing 2-(alkoxy)malonodinitriles from 2-alkoxymalondiamides
INVENTOR(S): Bartek, Johannes; Fuchs, Rudolf; Hildbrand, Stefan
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 13 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001058857	A1	20010816	WO 2001-EP1505	20010209

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, US, US, US, US
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

AU 2001033759	A5	20010820	AU 2001-33759		20010209
EP 1254105	A1	20021106	EP 2001-905765		20010209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2003522753	T2	20030729	JP 2001-558409		20010209
US 2003144538	A1	20030731	US 2002-182716		20021011
US 6673957	B2	20040106			
US 2004063987	A1	20040401	US 2003-673988		20030930
PRIORITY APPLN. INFO.:			EP 2000-102758	A	20000210
			EP 2000-109505	A	20000504
			US 2001-267087P	P	20010207
			WO 2001-EP1505	W	20010209
			US 2002-182716	A3	20021011

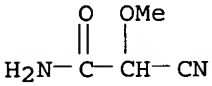
OTHER SOURCE(S): CASREACT 135:152562; MARPAT 135:152562

AB 2-(Alkoxy)malonodinitriles (NC)2CHOR (R = C1-6 alkyl, halogen-substituted C1-6 alkyl) (e.g., 2-methoxymalonodinitrile) or 2-(alkoxy)-2-cyanoacetamides are prepared by the dehydration of the corresponding 2-alkoxymalondiamides (H2NCO)2CHOR in the presence of a dehydrating agent (e.g., POCl3).

IT **353291-71-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(dehydration method for producing 2-(alkoxy)malonodinitriles from 2-alkoxymalondiamides)

RN 353291-71-1 HCAPLUS

CN Acetamide, 2-cyano-2-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:408241 HCAPLUS

DOCUMENT NUMBER: 115:8241

TITLE: Reactions of methoxynaphthalenes with active methylene compounds in the presence of manganese(III) acetate

AUTHOR(S): Tsunoda, Katsunori; Yamane, Mitsuyoshi; Nishino, Hiroshi; Kurosawa, Kazu

CORPORATE SOURCE: Fac. Sci., Kumamoto Univ., Kumamoto, 860, Japan

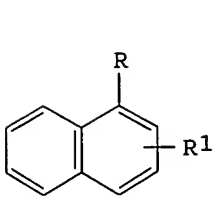
SOURCE: Bulletin of the Chemical Society of Japan (1991), 64(3), 851-6
CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

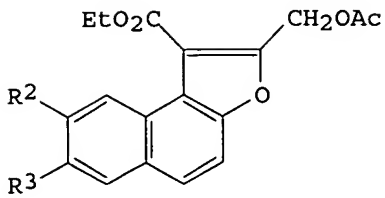
LANGUAGE: English

OTHER SOURCE(S): CASREACT 115:8241

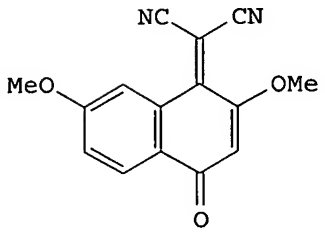
GI



I



II



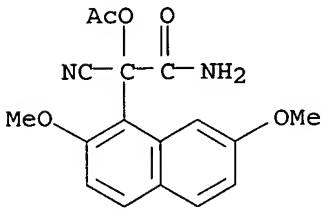
III

AB The reaction of methoxynaphthalenes I [R = H, R1 = 2-OMe, 4-OMe, 2,6-(OMe)2, 2,7-(OMe)2, 4,6-(OMe)2, 6,7-(OMe)2] with malonamide in the presence of manganese(III) acetate gave 2-acetoxy-2-(1-naphthyl)propanediamides I [R = C(OAc)(CONH2)2] and 2-hydroxy-2-(1-naphthyl)propanediamides I [R = C(OH)(CONH2)2]. The reaction of methoxynaphthalenes with Et 3-oxobutanoate, 2-cyanoacetamide, and malononitrile in the presence of manganese(III) acetate also yielded the corresponding substituted naphthalenes, Et 2-(acetoxymethyl)naphtho[furan-1-carboxylates II (R2, R3 = H, OMe), and/or a 4-methylnaphthalenone III. The reaction mechanisms are discussed.

IT **134255-39-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 134255-39-3 HCAPLUS

CN 1-Naphthaleneacetamide, α-(acetyloxy)-α-cyano-2,7-dimethoxy- (9CI) (CA INDEX NAME)



L12 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:579018 HCAPLUS

DOCUMENT NUMBER: 87:179018

TITLE: Amino acid derivatives as fungicides

INVENTOR(S): Ishida, Yasuo; Yakushiji, Kunito; Wakae, Osamu; Aoki, Isao; Masumoto, Keiichi

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

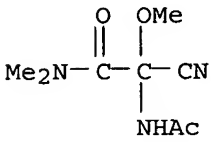
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52021327	A2	19770217	JP 1975-97931	19750811
PRIORITY APPLN. INFO.:			JP 1975-97931 A	19750811

AB Amino acid derivs. are used as microbicides. Thus, N,N,-dimethyl-2-acetamido-2-cyano-2-(propylthio)acetamide [PrSC(CN)(NHAc)CONMe2] [64205-24-9] sprayed on tomatoes at 250 ppm almost completely controlled Phytophthora infestans infection. This compound and 28 its analogs were prepared and their fungicidal activities presented.

IT **64205-28-3P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and fungicidal activity of)

RN 64205-28-3 HCAPLUS
CN Acetamide, 2-(acetylamino)-2-cyano-2-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)



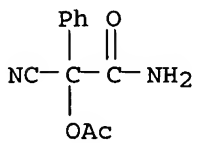
L12 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1968:12238 HCAPLUS
DOCUMENT NUMBER: 68:12238
TITLE: Cyanide-catalyzed fragmentation of triketone monoximes
AUTHOR(S): Crabtree, Eleanor V.; Poziomek, Edward J.
CORPORATE SOURCE: Edgewood Arsenal, Edgewood, MD, USA
SOURCE: Journal of Organic Chemistry (1967), 32(4), 1231-3
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB 1-Phenyl-1,2,3-butanetrione 2-oxime (I) is treated with KCN to give 2-cyano-2-hydroxy-2-phenylacetamide (II); N.M.R. data for II are given. The I-CN- reaction is inhibited by PhCOCONH2; CN- catalyzes the cleavage of I.

IT **7616-88-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

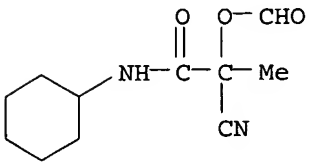
RN 7616-88-8 HCAPLUS
CN Mandelamide, α-cyano-, acetate (ester) (8CI) (CA INDEX NAME)



L12 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1966:465427 HCAPLUS
DOCUMENT NUMBER: 65:65427
ORIGINAL REFERENCE NO.: 65:12170c-e
TITLE: Heterocyclic isonitriles
AUTHOR(S): Neidlein, R.
CORPORATE SOURCE: Univ. Marburg/Lahn, Germany
SOURCE: Arch. Pharm (1966), 299(7), 603-5
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 65:65427

AB The preparation of 3-isonitrilopyridine (I) and α-furfurylisonitrile (II) and their reactions with carboxylic acids, ketones, and amines to give the corresponding acylaminocarboxamides are described. Acyl cyanides with isonitriles and carboxylic acids yielded the corresponding α-hydroxy-α-cyanocarboxamides. 3-Formamidopyridine (12.2 g.) in 32 cc. Et3N and 150 cc. CH2Cl2 treated with stirring and cooling with 9.9 g. COCl2 and then with 50 cc. saturated aqueous Na2CO3 yielded 7.3 g. I. N-Formyl-α-furfurylamine (12.5 g.), 32 cc. Et 3N, and 9.9 g. COCl2 gave similarly II. Cyclohexanone (5.4 g.) and 3.5 g. iso-PrNH2 treated slowly with cooling with 5.2 g. crude I in 25 cc. iso-PrOH and 2.6 cc. HCO2H and kept 4 hrs. gave 4.2 g. 1-(N-formylisopropylamino)cyclohexane-1-carboxylic acid 3-pyridylamide (III), m. 180-1° (MeCN). II (5.4 g.), 3.5 g. iso-PrNH2, and 54 g. cyclohexanone in 15 cc. PrOH treated at -30° with 2.6 g. HCO2H in portions yielded 4.5 g. α-furfurylamide analog of III, m. 137-8° (EtOH). Cyclohexyl isocyanide (5.45 g.) treated with cooling with 3.8 g. AcCN and then with 2.6 g. HCO2H in portions yielded 6.5 g. 2-cyano-2-formyloxypropionic acid cyclohexylamide, m. 123-4° (EtOH-petr. ether).

IT **91430-76-1**, Lactamide, 2-cyano-N-cyclohexyl-, formate (preparation of)
RN 91430-76-1 HCAPLUS
CN Lactamide, 2-cyano-N-cyclohexyl-, formate (7CI) (CA INDEX NAME)



L12 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1964:424911 HCAPLUS
DOCUMENT NUMBER: 61:24911
ORIGINAL REFERENCE NO.: 61:4210g-h,4211a-d
TITLE: Reactions between isonitrosoacetone and hydrocyanic acid
AUTHOR(S): Nenz, A.; Marangoni, L.; Gallinella, E.; Iliceto, A.
CORPORATE SOURCE: Soc. Edison, Milan
SOURCE: Chimica e l'Industria (Milan, Italy) (1964), 46(5), 509-17
CODEN: CINMAB; ISSN: 0009-4315
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 61:24911

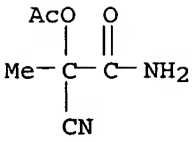
AB RCOCH:NOH (I) (R = Me), HCN, and a catalyst (piperidine, KOH, KCN, NaCN) were mixed at the rate 1:0.32:0.01 by weight, 5.5 parts of an inert solvent

(CCl4 or C2H4Cl2) added, the mixture kept in a closed vessel, with stirring, at 30°, 30-80 hrs., the solvent and residual HCN decanted or dist., the residue extracted with Et2O, and the resulting crude product recrystd. in CHCl3EtOH (95:5) to give RC(CN)(OH)CONH2 (II) (R = Me, IIa), m. 85-6°. In a similar way the following II were prepared [R, Hcn:I ratio, solvent, reaction temperature, time (hrs.), % yield, and m.p. given]: Et (III), 1, CCl4, 30°, 80, 39.6, 75-6°; iso-Bu (IV), 1, -, 30°, 70, 70.3, 84-5°; Ph (V), 2.4, CCl4, 20°, 190, 46.5, 91-2°; p-O2NC6H4 (VI), 2, CCl4, 20°, 140, 83.9, 149-50°. I (R = p-MeC6H4 and p-MeOC6H4) gave, under the same conditions, only p-MeC6H4CO2H and p-MeOC6H4CO2H, resp. MeC(CN)(OH)CH:NOH (VII) (5 g.) was kept at 30° in a closed vessel 4 days and taken up in 10 ml. Et2O and the solvent evaporated to give 2.8 g. crude IIa. To 5 g. VII in 20 ml. anhydrous Et2O 1.8 g. HCl gas was introduced at -15% the mixture kept at this temperature 3 hrs., the solvent evaporated, and the product dried at -25° during 4 hrs. to give 3.2 g. IIa. AcCONH2 (5 g.) was added with stirring to a mixture of 27 g. CCl4, 1.6 g. HCN, and 0.05 g. piperidine, after 5 min. the solvent was evaporated, a few ml. Et2O and 40 ml. boiling CHCl3 added, and the mixture worked up to give 3 g. IIa. II (10 g.) was dissolved in 62 g. 97.2% H2SO4, at 0-20° and kept overnight at room temperature, the solution poured into 500 ml. Et2O, the precipitate taken up in 70 ml. EtOH, and the solution worked up to give 9.4 g. MeC(OH)(CONH2)2 (VIII), m. 211-12°. IIa (10 g.) was dissolved in 20 ml. concentrated HCl, keeping the temperature below 65°, left overnight at room temperature, and extracted 10 times with 50 ml. Et2O, and the solution worked up to give 6.2 g. MeC(OH)(CO2H)2 (IX), m. 140° (H2O). IIa (10 g.) was dissolved in 17 g. 100% H2SO4, keeping the temperature below 60°, heated 1 hr. at 100°, and cooled to 60°, 11.2 g. MeOH added, the mixture heated 15 hrs. at 90°, 60 ml. anhydrous Et2O added, and the solution worked up to give 9.7 g. MeC(OH)(CO2Me)2 (X), b3 71°, n20D 1.4287. To 30 g. IIa in 100 ml. Ac2O, 0.1 g. C5H5N was added and the mixture heated 100 min. at 90°, cooled below 50°, and distilled in vacuo until dryness; the residue was taken up in C6H6 to give 38.8 g. MeC(OAc)(CN)CONH2 (XI), m. 98-9° (AcOEt). A solution of 20 g. IIa in 200 ml. anhydrous C5H5N was treated at 0° with 20 g. ClSO3H, the mixture kept overnight, with stirring, at room temperature and cooled to 0°, 42 g. NaHCO3 added, stirring continued 3 hrs., the mixture filtered, the solution evaporated in vacuo to dryness, keeping the temperature below 30°, and the residue taken up in 100 ml. absolute EtOH to give 28.8 g. C5H5N salt of MeC(OSO3H)(CN)CONH2 (XII), m. 130-1° (MeOH). XII was dissolved in MeOH and treated with MeONa to give the corresponding Na salt, m. 185-7°. Through a solution of 20 g. IIa in 50 ml. MeOH, cooled at 5°, dry NH3 gas was slowly passed during 12 hrs., the precipitated solid filtered off, the solution evapd, in vacuo to dryness, and the residue taken up in 20 ml. absolute EtOH, to give 9.5 g. MeC(NH2)(CN)CONH2 (XIII), m. 110-2° (C2H4Cl2). The infrared spectra of III, IV, V, VI, VIII, IX, X, XI, XII, and XIII were given. The probable reaction mechanism as it results from the use of H14CN was discussed.

IT **89532-92-3**, Lactamide, 2-cyano-, acetate (ester)
(preparation of)

RN 89532-92-3 HCAPLUS

CN Lactamide, 2-cyano-, acetate (7CI) (CA INDEX NAME)



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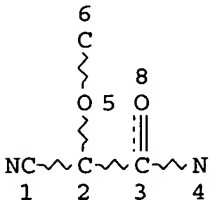

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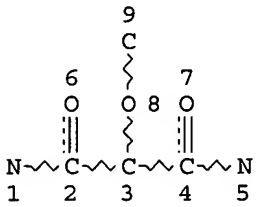

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L13            70 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8
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L23  ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2005:220131  HCAPLUS
DOCUMENT NUMBER:          142:298014
TITLE:                    Preparation of dibenzoazepinylmalonamides,
                          dibenzooxepinylmalonamides,
                          benzodiazepinylmalonamides, and related compounds as
                          γ-secretase inhibitors for treatment of
                          Alzheimer's disease.
INVENTOR(S):              Flohr, Alexander; Galley, Guido; Jakob-Roetne, Roland;
                          Kitas, Eric Argirios; Peters, Jens-Uwe; Wostl,
                          Wolfgang
PATENT ASSIGNEE(S):       Switz.
SOURCE:                   U.S. Pat. Appl. Publ., 59 pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
     US 2005054633         A1    20050310    US 2004-933177          20040902
     WO 2005023772         A1    20050317    WO 2004-EP9700          20040831
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
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             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
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PRIORITY APPLN. INFO.:                       EP 2003-19683       A  20030909
OTHER SOURCE(S):          MARPAT 142:298014
GI
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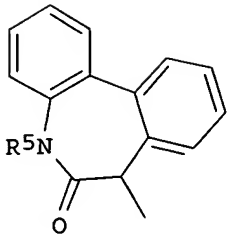
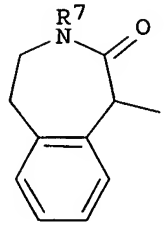
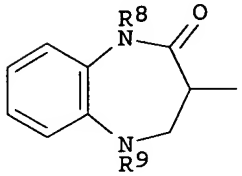
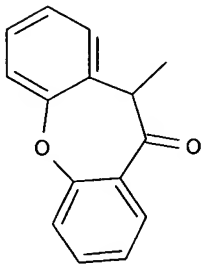
Q1 = 

Q2 = 

Q3 = 

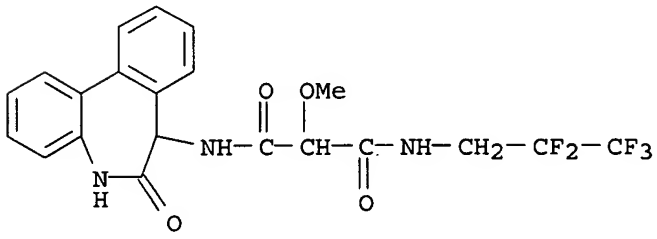
Q4 = 

AB Malonamides R1NHCOCR3R4CONHR2 [R1= Q1-Q4; R2 = alkyl, alkynyl, alkylthio, alkoxy(alkyl), halo(alkyl), etc.; R3, R4 = H, alkyl, alkoxy, Ph, halo; R5 = H, alkyl, trifluoromethyl(alkyl), cycloalkyl(alkyl); R6 = H, halo; R7 = H, alkyl; R8 = H, alkyl, alkynyl, trifluoromethyl(alkyl), cycloalkyl(alkyl), (halo-substituted) phenyl(alkyl); R9 = H, alkyl, CHO, alkylcarbonyl, F3CCO, (substituted) PhCO, etc.], were prepared Thus, 2-methyl-N-(5-methyl-6-oxo-6,7-dihydro-5H-dibenzo[b,d]azepin-7-yl)malonamic acid (preparation given), cyclopropylmethylamine, and 2-(2-pyridon-1-yl)-1,1,3,3-tetramethyluronium tetrafluoroborate (TPTU) were shaken together overnight in DMF to give N-cyclopropylmethyl-2-methyl-N'-(5-methyl-6-oxo-6,7-dihydro-5H-dibenzo[b,d]azepin-7-yl)malonamide. The latter inhibited γ-secretase with IC50 = 0.09 μM.

IT **847925-92-2P 847926-00-5P 847926-11-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of dibenzoazepinylmalonamides, dibenzooxepinylmalonamides, benzodiazepinylmalonamides, and related compds. as γ-secretase inhibitors for treatment of Alzheimer's disease)

RN 847925-92-2 HCAPLUS

CN Propanediamide, N-(6,7-dihydro-6-oxo-5H-dibenz[b,d]azepin-7-yl)-2-methoxy-N'-(2,2,3,3,3-pentafluoropropyl)- (9CI) (CA INDEX NAME)

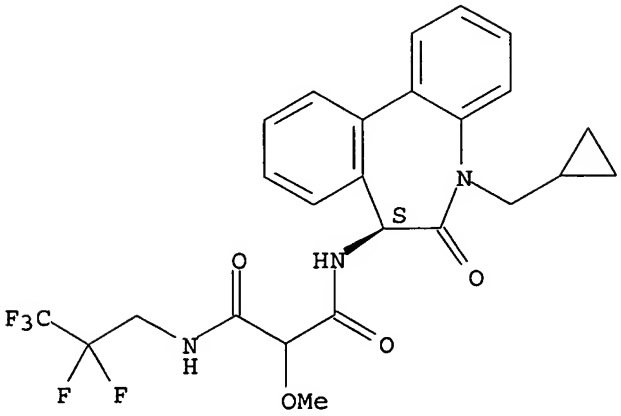


RN 847926-00-5 HCAPLUS

CN Propanediamide, N-[(7S)-5-(cyclopropylmethyl)-6,7-dihydro-6-oxo-5H-

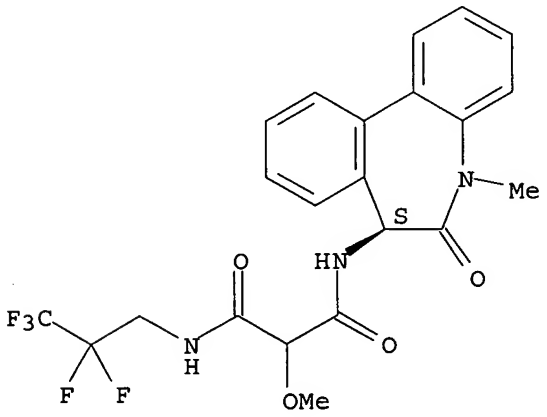
dibenz[b,d]azepin-7-yl]-2-methoxy-N'-(2,2,3,3,3-pentafluoropropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



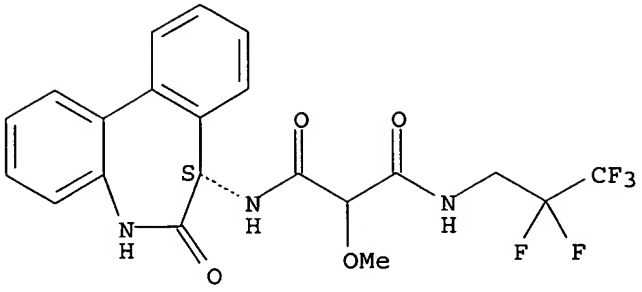
RN 847926-11-8 HCAPLUS
CN Propanediamide, N-[(7S)-6,7-dihydro-5-methyl-6-oxo-5H-dibenz[b,d]azepin-7-yl]-2-methoxy-N'-(2,2,3,3,3-pentafluoropropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

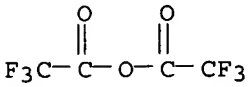


IT **847927-37-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dibenzoazepinylmalonamides, dibenzooxepinylmalonamides, benzodiazepinylmalonamides, and related compds. as γ-secretase inhibitors for treatment of Alzheimer's disease)
RN 847927-37-1 HCAPLUS
CN Propanediamide, N-[(7S)-6,7-dihydro-6-oxo-5H-dibenz[b,d]azepin-7-yl]-2-methoxy-N'-(2,2,3,3,3-pentafluoropropyl)- (9CI) (CA INDEX NAME)

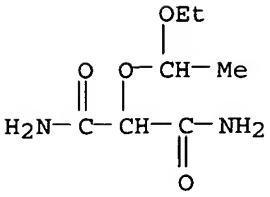
Absolute stereochemistry.



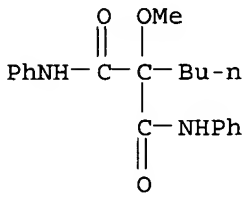
IT **407-25-0, Trifluoroacetic anhydride**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of dibenzoazepinylmalonamides, dibenzooxepinylmalonamides, benzodiazepinylmalonamides, and related compds. as γ-secretase inhibitors for treatment of Alzheimer's disease)
RN 407-25-0 HCAPLUS
CN Acetic acid, trifluoro-, anhydride (6CI, 8CI, 9CI) (CA INDEX NAME)



L23 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:478964 HCAPLUS
DOCUMENT NUMBER: 113:78964
TITLE: Development of a new acyl anion equivalent for the preparation of masked activated esters, and their use to prepare a dipeptide
AUTHOR(S): Nemoto, Hisao; Kubota, Yasufumi; Yamamoto, Yoshinori
CORPORATE SOURCE: Fac. Sci., Tohoku Univ., Sendai, 980, Japan
SOURCE: Journal of Organic Chemistry (1990), 55(15), 4515-16
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:78964
AB New acyl anion equivs., the protected hydroxymalonitriles ROCH(CN)2 (I, R = CHMeOEt, SiMe2CMe3) have been developed as masked activated ester equivs. Alkylation or allylation of I (R = CHMeOEt) proceeded in high yields under mild basic or neutral conditions, resp. Treatment of the tosylimine 4-MeOC6H4CH:NSO2C6H4Me-4 with I (R = CHMeOEt) gave the dipeptide 4-MeOC6H4CHR1NR2SO2C6H4Me-4 (II, R1 = CO-Gly-OMe, R2 = CH2OMe) via the α-amino acid II [R1 = C(CN)2OCHMeOEt, R2 = H] having a masked activated functionality.
IT **128326-92-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and **dehydration** of, malononitrile derivative from)
RN 128326-92-1 HCAPLUS
CN Propanediamide, 2-(1-ethoxyethoxy)- (9CI) (CA INDEX NAME)



L23 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1974:437004 HCAPLUS
DOCUMENT NUMBER: 81:37004
TITLE: Light induced reactions of 4-n-butyl-1,2-diphenylpyrazolidine-3,5-dione (phenylbutazone) with nucleophilic agents
AUTHOR(S): Reisch, J.; Weidmann, K. G.; Triebe, J.
CORPORATE SOURCE: Inst. Pharm. Chem., Westfael. Wilhelms-Univ. Muenster, Muenster/Westf., Fed. Rep. Ger.
SOURCE: Experientia (1974), 30(5), 451-2
CODEN: EXPEAM; ISSN: 0014-4754
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Uv irradiation of phenylbutazone (I) forms an aziridinone intermediate (II), which in the presence of MeOH or Me2NH gives PhNHCOCBuRCONHPh (III; R = MeO, Me2N). In H2O solution II forms III (R = OH), which is **dehydrated** to PhNHCOC(:CHPr)CONHPr or decomps. to HCONHPh and PhNH2.
IT **52884-93-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 52884-93-2 HCAPLUS
CN Propanediamide, 2-butyl-2-methoxy-N,N'-diphenyl- (9CI) (CA INDEX NAME)



L23 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1973:84132 HCAPLUS
DOCUMENT NUMBER: 78:84132
TITLE: Reaction of aliphatic isocyanides with chloroacetic anhydride and **trifluoroacetic anhydride**
AUTHOR(S): Krivinka, P.; Honzl, J.
CORPORATE SOURCE: Cesk. Akad. Ved, Prague, Czech.
SOURCE: Collection of Czechoslovak Chemical Communications (1972), 37(12), 4035-40
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: English

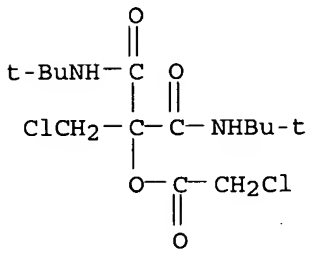
GI For diagram(s), see printed CA Issue.

AB MeNC (I) and (ClCH2CO)2O (II) in CHCl3 at 30° gave ClCH2(CO)2NMeCOCH2Cl which was converted in aqueous tetrahydrofuran to ClCH2C(OH)2CONMeCOCH2Cl. Reaction of I and (F3CCO)2O (III) in CCl4 and hydrolysis gave F3CC(OH)2CONHMe. Reaction of tert-BuNC (IV) and II in CHCl3 and hydrolysis gave (tert-BuNHCO)2C(CH2Cl)OCOCH2Cl (V). V kept in liquid NH3 gave (tert-BuNHCO)2C(CH2Cl)OH. Reduction of V with activated Al in aqueous tetrahydrofuran gave (tert-BuNHCO)2C(CH2Cl)OAc. Reaction of III and IV in CCl4 at 0° and decomposition with H2O gave (tert-BuNHCO)2C(OH)CF3 (VI); decomposition with EtOH gave 1-tert-butyl-3-hydroxy-3-(trifluoromethyl)-4-(tert-butylimino)-2-azetidinone (VII). Acetylation of VI (Ac2O-pyridine) or VII [Pb(OAc)4] gave (tert-BuNHCO)2C(OAc)CF3.

IT **39528-85-3P 39528-87-5P 39528-90-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

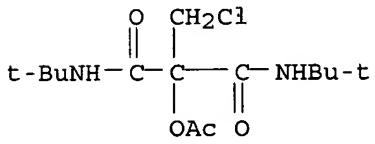
RN 39528-85-3 HCAPLUS

CN Acetic acid, chloro-, 1-(chloromethyl)-2-[(1,1-dimethylethyl)amino]-1-[[(1,1-dimethylethyl)amino]carbonyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)



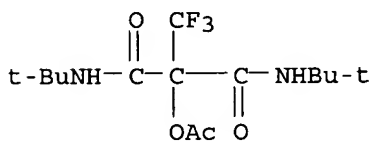
RN 39528-87-5 HCAPLUS

CN Propanediamide, 2-(acetyloxy)-2-(chloromethyl)-N,N'-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



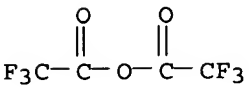
RN 39528-90-0 HCAPLUS

CN Propanediamide, 2-(acetyloxy)-N,N'-bis(1,1-dimethylethyl)-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)

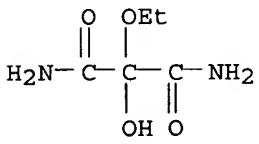


IT **407-25-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with alkyl isocyanides)

RN 407-25-0 HCAPLUS
CN Acetic acid, trifluoro-, anhydride (6CI, 8CI, 9CI) (CA INDEX NAME)



L23 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1964:432402 HCAPLUS
DOCUMENT NUMBER: 61:32402
ORIGINAL REFERENCE NO.: 61:5639f-h
TITLE: Hydroxy-1,2,5-thiadiazoles. I. A novel route from potassium cyanide and sulfur dioxide
AUTHOR(S): Ross, John M.; Smith, William C.
CORPORATE SOURCE: E. I. du Pont de Nemours & Co. Inc., Wilmington, DE
SOURCE: Journal of the American Chemical Society (1964), 86(14), 2861-8
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 61:32402
GI For diagram(s), see printed CA Issue.
AB 3-**Cyano**-4-hydroxy-1,2,5-thiadiazole (I) has been obtained from the reaction of KCN and SO2 at 25-85° in the absence of hydroxylic solvents. The structure was elucidated by degradation to **diethylaminoacetamide** and to N-sulfamoyloxamic acid dipotassium salt, and by independent synthesis from **isonitrosocyanoacetamide** and S2Cl2. Various 3-hydroxy-1,2,5-thiadiazole derivs. were prepared including several K acid salts involving sym. Hbonding of the acidic 3-hydroxy proton.
IT **89799-70-2**, Tartronamide, 2-ethoxy-
(preparation of)
RN 89799-70-2 HCAPLUS
CN Tartronamide, 2-ethoxy- (7CI) (CA INDEX NAME)



=> => d stat que l27 nos
L1 STR
L3 31 SEA FILE=REGISTRY SSS FUL L1
L6 STR
L8 158 SEA FILE=REGISTRY SSS FUL L6
L9 49 SEA FILE=REGISTRY ABB=ON PLU=ON TRIFLUOROACETIC ANHYDRIDE?/CN OR DIBUTYLTIN OXIDE?/CN OR PHOSPHORUS OXYCHLORIDE?/CN OR PHOSPHORUS TRICHLORIDE?/CN OR PHOSPHORUS PENTACHLORIDE?/CN
L11 643 SEA FILE=REGISTRY ABB=ON PLU=ON ALUMINUM CHLORIDE?/CN
L12 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L3
L14 25437 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 OR TRIFLUOROACETIC(W)ANHYDRIDE OR DIBUTYLTIN(W) OXIDE OR PHOSPHORUS(W)(OXYCHLORIDE? OR

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               TRICHLORIDE OR PENTACHLORIDE?)
L15        73122 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11 OR ALUMINUM (W)CHLORIDE
               OR ALCL3
L16       389244 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("DEHYDRATION AGENTS"/CV OR
               "DEHYDRATION REACTION (L) AGENTS"/CV OR "DRYING AGENTS"/CV) OR
               DEHYDRAT? OR DRYING
L17        30094 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("LEWIS ACIDS"/CV OR "CARBONYL
               S (L) LEWIS ACID COMPLEXES"/CV OR "CHARGE TRANSFER COMPLEXES"/C
               V OR ELECTROPHILES/CV OR "LEWIS ACIDITY"/CV OR "LEWIS BASES"/CV
               ) OR LEWIS(W)ACID
L20            4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L8 AND (L16 OR L14 OR L17 OR
               L15)) NOT L12
L26           15 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "HILDBRAND STEFAN"/AU
L27           14 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L26 NOT (L12 OR L20)


=> d ibib abs l27 1-14

L27  ANSWER 1 OF 14  HCAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2003:221642  HCAPLUS
DOCUMENT NUMBER:          138:238184
TITLE:                    Amidation and hydrogenation method for producing
                          beta-alanine amides from amines and cyanoacetate
                          esters
INVENTOR(S):              Hanselmann, Paul; Hildbrand, Stefan
PATENT ASSIGNEE(S):       Lonza A.-G., Switz.
SOURCE:                   PCT Int. Appl., 21 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 German
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
     WO 2003022795         A1    20030320    WO 2002-EP9893          20020904
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD,
             RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
     EP 1430018            A1    20040623    EP 2002-767473          20020904
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
     JP 2005502697         T2    20050127    JP 2003-526873          20020904
     US 2004220410         A1    20041104    US 2004-488692          20040305
PRIORITY APPLN. INFO.:                       EP 2001-121342      A   20010906
                                             US 2001-332547P     P   20011126
                                             WO 2002-EP9893      W   20020904
OTHER SOURCE(S):          CASREACT 138:238184; MARPAT 138:238184
AB   β-Alanine amides R2(R1CH2)NCOCH2CH2NH2 [R1 = H, (un)substituted C1-6
     alkyl; R2 = H; R1R2 = (CH2)n; n = 3, 4; e.g., carcinine], used as an
     active ingredient having an antioxidative effect in medicaments and
     cosmetics (no data), are produced without using an amino protective group
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by the amidation of the corresponding amine R2(R1CH2)NH (e.g., histamine) with a cyanoacetic ester R3O2CCH2CN (R3 = C1-10 alkyl; e.g., Et cyanoacetate) in order to form a cyanoacetamide R2(R1CH2)NCOCH2CN [e.g., 2-Cyano-N-[2-(1(3)H-imidazol-4-yl)ethyl]acetamide] and by subjecting the cyanoacetamide to catalytic hydrogenation.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:661387 HCAPLUS
DOCUMENT NUMBER: 135:211285
TITLE: Preparation of β-alaninamide dipeptides from N-unprotected amino acids or esters and cyanoacetic acid derivatives
INVENTOR(S): **Hildbrand, Stefan**; Ruppen, Thomas; Veghini, Dario
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2001064638	A1	20010907	WO 2001-EP2349		20010302
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, US, US, US, US					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
EP 1259483	A1	20021127	EP 2001-936057		20010302
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2004509834	T2	20040402	JP 2001-563481		20010302
US 2003105335	A1	20030605	US 2002-220608		20021121
US 6878829	B2	20050412			
US 2005192354	A1	20050901	US 2005-102828		20050411
PRIORITY APPLN. INFO.:			EP 2000-104643	A	20000303
			US 2001-271694P	P	20010228
			WO 2001-EP2349	W	20010302
			US 2002-220608	A3	20021121

OTHER SOURCE(S): CASREACT 135:211285; MARPAT 135:211285

AB The invention relates to β-alaninamides of general formula H2N(CH2)2C(O)N(R2)CH(R1)C(O)OR [R = H, a neg. charge compensated for by an equivalent of an inorg. or organic cation, or alkyl; R1 = H, (substituted) alkyl; R2 = H, or R1 and R2, together, form a group of formula -(CH2)n; n = 3 or 4]. The β-alaninamides are produced without using an amino protective group by reacting the corresponding α-amino acid or the corresponding α-amino acid ester with a cyanoacetic acid to form a cyanoacetic acid amide and by a subsequent catalytic hydrogenation. The method is particularly suited for producing carnosine (β-alanyl-L-histidine), a naturally occurring dipeptide, which is used as a food additive having an antioxidant effect. Thus, cyanoacetic acid Et ester

was coupled to L-histidine and the resulting dipeptide hydrogenated using a rhodium catalyst to give L-carnosine (76% yield, 99.5% optical purity). Anserin (β-alanyl-3-methyl-L-histidine) was similarly prepared, in 45% yield, starting from 3-methyl-L-histidine and cyanoacetic acid Et ester.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:564992 HCAPLUS
DOCUMENT NUMBER: 135:122023
TITLE: Amidation and etherification method for producing N-alkoxy-N-alkylcarboxamides from carboxylate esters
INVENTOR(S): Hanselmann, Paul; **Hildbrand, Stefan**; Sterren, Etienne
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 17 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001055096	A1	20010802	WO 2001-EP753	20010124
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, US, US				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1250316	A1	20021023	EP 2001-913765	20010124
EP 1250316	B1	20041229		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003520844	T2	20030708	JP 2001-555038	20010124
AT 286020	E	20050115	AT 2001-913765	20010124
US 2004030142	A1	20040212	US 2002-181420	20020724
US 6891049	B2	20050510		

PRIORITY APPLN. INFO.:

EP 2000-101391	A	20000125
US 2000-203906P	P	20000512
WO 2001-EP753	W	20010124

OTHER SOURCE(S): CASREACT 135:122023; MARPAT 135:122023

AB N-alkoxy-N-alkylcarboxamides R1CON(R2)(OR2) (R1 = C1-10 alkyl, cycloalkyl, cycloalkenyl, C2-10 alkenyl, aryl, arylalkyl, heteroaryl, heteroarylalkyl, heterocyclyl; R2 = C1-6 alkyl) (e.g., N-methoxy-N-methyl-2-furancarboxamide) are prepared in high yield and selectivity by the amidation of carboxylate esters R1COOR3 (R3 = C1-6 alkyl, 4-nitrophenyl, 2,4-dinitrophenyl, succinimido, benzotriazole-1-yl) (e.g., Me 2-furancarboxylate) with hydroxylamine, a hydroxylamine derivative, or with a hydroxylammonium salt (e.g., hydroxylammonium sulfate), and the reaction product is alkylated and etherified with R2X (X = halogen) (e.g., chloromethane) in the presence of a phase-transfer catalyst (e.g., tetrabutylammonium bromide).

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:167957 HCAPLUS
DOCUMENT NUMBER: 134:207549
TITLE: Oxidative method and catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles
INVENTOR(S): Hanselmann, Paul; **Hildbrand, Stefan**
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001016092	A1	20010308	WO 2000-EP8397	20000829
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1208081	A1	20020529	EP 2000-964050	20000829
EP 1208081	B1	20040414		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003532628	T2	20031105	JP 2001-519662	20000829
AT 264296	E	20040415	AT 2000-964050	20000829
ES 2219396	T3	20041201	ES 2000-964050	20000829
TW 572875	B	20040121	TW 2000-89127179	20001219
US 6700010	B1	20040302	US 2002-69579	20020712
HK 1048107	A1	20050527	HK 2003-100196	20030108

PRIORITY APPLN. INFO.:
EP 1999-117033 A 19990830
US 2000-185372P P 20000228
WO 2000-EP8397 W 20000829

OTHER SOURCE(S): CASREACT 134:207549; MARPAT 134:207549
AB Cyanoacetate esters NCCH2CO2R [R = (un)substituted (un)branched C1-8 alkyl, arylalkyl] (e.g., Me 2-cyanoacetate) are prepared in high yield and selectivity by the oxidation of 3-(alkoxy)propionitriles RO(CH2)2CN (e.g., 3-methoxypropionitrile) in the presence of a catalyst based on lead or on one of the transition metals (e.g., cobalt diacetate tetrahydrate) using oxygen or an oxygen-forming reagent (e.g., N-hydroxyphthalimide).
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:573541 HCAPLUS
DOCUMENT NUMBER: 133:164469
TITLE: Preparation of cyanoacetate esters
INVENTOR(S): Hanselmann, Paul; **Hildbrand, Stefan**
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: Eur. Pat. Appl., 5 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1028105	A1	20000816	EP 2000-102087	20000203
EP 1028105	B1	20040421		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
IL 134110	A1	20041215	IL 2000-134110	20000118
TW 526186	B	20030401	TW 2000-89100864	20000120
KR 2000057793	A	20000925	KR 2000-3077	20000122
CN 1266845	A	20000920	CN 2000-101944	20000131
CA 2297636	AA	20000809	CA 2000-2297636	20000203
AT 264836	E	20040515	AT 2000-102087	20000203
PT 1028105	T	20040930	PT 2000-102087	20000203
ES 2220265	T3	20041216	ES 2000-102087	20000203
JP 2000229930	A2	20000822	JP 2000-27076	20000204
NO 2000000625	A	20000810	NO 2000-625	20000208
US 6239307	B1	20010529	US 2000-500634	20000209
HK 1030205	A1	20041119	HK 2001-101240	20010221
PRIORITY APPLN. INFO.:			EP 1999-102286 A	19990209
			US 1999-145997P P	19990729

OTHER SOURCE(S): MARPAT 133:164469

AB In the title process, in which aqueous NCCH2CO2Na solns. can be esterified directly, the alkali cyanoacetate solution is treated with alkyl, alkenyl, or aryl halides in 2-phase H2O-organic systems in the presence of phase-transfer catalysts. Adding 0.20 mol MeCl to a mixture of 0.02 mol NCCH2CO2H, 0.02 mol NaOH, 2.0 mmol Bu4N+ Br-, and 15 mL 2:1 tert-BuOMe-H2O, heating over 30 min to 100°, and holding at 100°/10 bar for 3.5 h gave 68% NCCH2CO2Me.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:501822 HCAPLUS
DOCUMENT NUMBER: 133:89232
TITLE: Preparation of malonic esters
INVENTOR(S): **Hildbrand, Stefan**; Hanselmann, Paul
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000204061	A2	20000725	JP 2000-1898	20000107
EP 1026148	A1	20000809	EP 2000-100310	20000107
EP 1026148	B1	20030507		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
AT 239692	E	20030515	AT 2000-100310	20000107
PT 1026148	T	20030930	PT 2000-100310	20000107
SK 283638	B6	20031104	SK 2000-24	20000107
ES 2199100	T3	20040216	ES 2000-100310	20000107
NO 2000000109	A	20000712	NO 2000-109	20000110
NO 314757	B1	20030519		
KR 2000053438	A	20000825	KR 2000-896	20000110

US 6350898	B1	20020226	US 2000-480165	20000110
CN 1263885	A	20000823	CN 2000-101055	20000111

PRIORITY APPLN. INFO.: EP 1999-100411 A 19990111
OTHER SOURCE(S): CASREACT 133:89232; MARPAT 133:89232
AB Title compds. CH2(CO2R)2 (R = alkyl, alkenyl, arylalkyl) are prepared by reaction of alkali salts of malonic acid with RX (X = halo) in water in the presence of phase transfer catalysts. Thus, reaction of disodium malonate with MeCl in H2O in the presence of Bu4NBr at 100° for 3 h gave 48% di-Me malonate.

L27 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:384137 HCAPLUS
DOCUMENT NUMBER: 133:32023
TITLE: Manufacture of hydroxamic acid esters in one-pot amidation-alkylation of corresponding esters
INVENTOR(S): Hanselmann, Paul; **Hildbrand, Stefan**
PATENT ASSIGNEE(S): Lonza AG, Switz.
SOURCE: PCT Int. Appl., 15 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000032564	A1	20000608	WO 1999-EP9121	19991125

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: EP 1998-122927 A 19981203
OTHER SOURCE(S): MARPAT 133:32023
AB Hydroxamic acid esters are manufactured in a one-pot process involving aqueous reaction of a corresponding ester with a hydroxylammonium salt (typically hydroxylamine hydrochloride or hydroxylamine sulfate) in the presence of strong base, followed by base-catalyzed alkylation with a dialkyl sulfate or an alkyl chloride. The intermediate hydroxy amides are not isolated; the product O-alkyl hydroxamic esters is prepared in high yield with minimal content of N,O-dialkylated byproducts. The hydroxamic acid esters have the general formula R1R2C=C(R3)-C(:O)-NH-OR, which are derived from the corresponding esters, of general formula R1R2C=C(R3)-C(:O)-O-R' (R = C1-6-alkyl; R1-3 = H or C1-4-alkyl; and R' = C1-6-alkyl). Alkylation is carried out using, as alkylating agents, a dialkyl sulfate, (RO)2SO2, or an alkyl chloride, RCl (R = C1-6-alkyl). The hydroxamic acid ester are suitable as blocking agents for isocyanates.
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:680946 HCAPLUS
DOCUMENT NUMBER: 132:78124
TITLE: Regio- and enantioselective molybdenum-catalyzed alkylations of polyenyl esters
AUTHOR(S): Trost, Barry M.; **Hildbrand, Stefan**; Dogra,

Kalindi
CORPORATE SOURCE: Department of Chemistry, Stanford University, Stanford, CA, 94305-5080, USA
SOURCE: Journal of the American Chemical Society (1999), 121(44), 10416-10417
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:78124
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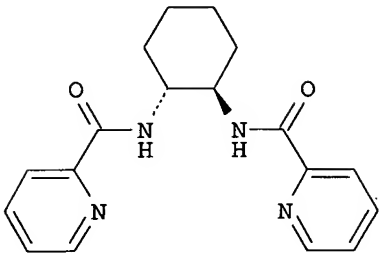

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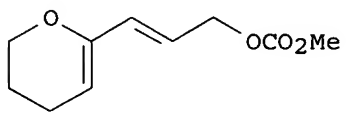

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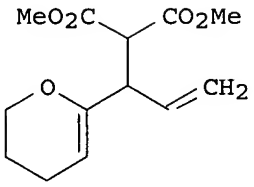


IV

AB The title reaction was examined using (EtCN)3Mo(CO)3 (I) as catalyst and several diamine ligands. Thus, reacting PhCH:CHCH:CHCH2OCO2Me with (MeO2C)2CH using I and diamine II gave (MeO2C)2CC(CH:CH2)CH:CHPh in 98% ee. Polyenyl carbonate III gave diester IV in 96% ee after 1.5 h.
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:272282 HCAPLUS
DOCUMENT NUMBER: 129:51267
TITLE: Inhibition of DNA polymerase reactions by pyrimidine nucleotide analogs lacking the 2-keto group
AUTHOR(S): Guo, Mao-Jun; **Hildbrand, Stefan**; Leumann, Christian J.; Mclaughlin, Larry W.; Waring, Michael J.
CORPORATE SOURCE: Department of Pharmacology, University of Cambridge, Cambridge, CB2 1QJ, UK
SOURCE: Nucleic Acids Research (1998), 26(8), 1863-1869
CODEN: NARHAD; ISSN: 0305-1048
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB To investigate the influence of the pyrimidine 2-keto group on selection

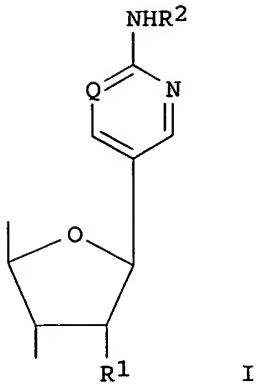
of nucleotides for incorporation into DNA by polymerases, we have prepared two C nucleoside triphosphates that are analogs of dCTP and dTTP, namely 2-amino-5-(2'-deoxy-β-D-ribofuranosyl)pyridine-5'-triphosphate (d*CTP) and 5-(2'-deoxy-β-D-ribofuranosyl)-3-methyl-2-pyridone-5'-triphosphate (d*TTP) resp. Both proved strongly inhibitory to PCR catalyzed by Taq polymerase; d*TTP rather more so than d*CTP. In primer extension expts. conducted with either Taq polymerase or the Klenow fragment of Escherichia coli DNA polymerase I, both nucleotides failed to substitute for their natural pyrimidine counterparts. Neither derivative was incorporated as a chain terminator. Their capacity to inhibit DNA polymerase activity may well result from incompatibility with the correctly folded form of the polymerase enzyme needed to stabilize the transition state and catalyze phosphodiester bond formation.

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:740245 HCAPLUS
DOCUMENT NUMBER: 127:346619
TITLE: Preparation of modified cytidine-containing oligodeoxyribonucleotide triplexes
INVENTOR(S): Leumann, Christian; **Hildbrand, Stefan**
PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Leumann, Christian; Hildebrand, Stefan
SOURCE: PCT Int. Appl., 72 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9741140	A1	19971106	WO 1997-EP1856	19970414
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9726968	A1	19971119	AU 1997-26968	19970414
PRIORITY APPLN. INFO.:			CH 1996-1059 A	19960426
			WO 1997-EP1856 W	19970414

OTHER SOURCE(S): MARPAT 127:346619
GI



I

AB Oligodeoxyribonucleotide in which at least one cytidine building block is replaced with an analogous building block I [Q = N, CR; R = H, alkyl; R1 = H, (un)substituted alkyl, alkoxy, oxymethyl-heterocycle; R2 = H, alkyl, aminoalkyl, alkylamino, alkoxyalkyl] in which the cytidine residue is replaced with a C-bonded aminopyridyl or aminopyrimidyl were prepared Affinity and interaction of these oligodeoxyribonucleotides with DNA duplexes is reported. Thermal stability and hyperchromicity of these DNA triplexes are reported.

L27 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:347278 HCAPLUS
DOCUMENT NUMBER: 127:66082
TITLE: 5-Substituted 2-Aminopyridine C-Nucleosides as Protonated Cytidine Equivalents: Increasing Efficiency and Specificity in DNA Triple-Helix Formation
AUTHOR(S): **Hildbrand, Stefan**; Blaser, Adrian; Parel, Serge P.; Leumann, Christian J.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Bern, Bern, CH-3012, Switz.
SOURCE: Journal of the American Chemical Society (1997), 119(24), 5499-5511
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The easily accessible C-nucleoside 2-amino-5-(2'-deoxy-β-D-ribofuranosyl)pyridine (P) and its 3-Me (X) and 2'-O-Me (Y) derivs. were synthesized and incorporated as protonated cytidine equivalent in homopyrimidine oligodeoxyribonucleotides. Tm measurements indicate that oligodeoxyribonucleotides containing P or X have a higher affinity to double-stranded DNA over the pH range of 6-8 than 5-methylcytidine (Z) containing oligodeoxyribonucleotides. This increase in stability is most pronounced above pH 7.0. The average increase in Tm/modification for the dissociation of oligodeoxyribonucleotide d(TTTTTXTXTXTXTXT) from a 21-mer target duplex at pH 7.5 is 2.3 °C relative to oligodeoxyribonucleotide d(TTTTTZTZTZTZTZT). The pH dependence and sequence composition effects are much less pronounced for X (and also P) containing oligodeoxyribonucleotides than for Z containing ones. While oligodeoxyribonucleotide d(TTTZZZZTTTTZTTT) has already no longer any affinity to the target duplex above pH 6.5, oligodeoxyribonucleotide d(TTTXXXXTTTTXTTT) displays preserved binding with a Tm of 32.5 °C

at pH 7.0 and even binds with a Tm of 23.3 °C at pH 8.0. The average decrease in Tm/modification for oligodeoxyribonucleotide d(TTTTTYTYTYTYTYT) at pH 6.5 is 6.7 °C relative to the Z containing oligodeoxyribonucleotide. DNase I footprint titration expts. indicate that d(TTTTTXTXTXTXTXT) binds not only five times stronger to a 229 base pair DNA fragment than d(TTTTTZTZTZTZTZT) but also with higher selectivity. Thus the new bases P and X show Hoogsteen specific pairing behavior.

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:595218 HCAPLUS
DOCUMENT NUMBER: 126:8456
TITLE: Enhancing DNA triple helix stability at neutral pH by the use of oligonucleotides containing a more basic deoxycytidine analog.
AUTHOR(S): **Hildbrand, Stefan**; Leumann, Christian
CORPORATE SOURCE: Inst. organische, Chemie der Univ., Bern, CH-3012, Switz.
SOURCE: Angewandte Chemie, International Edition in English (1996), 35(17), 1968-1970
CODEN: ACIEAY; ISSN: 0570-0833
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
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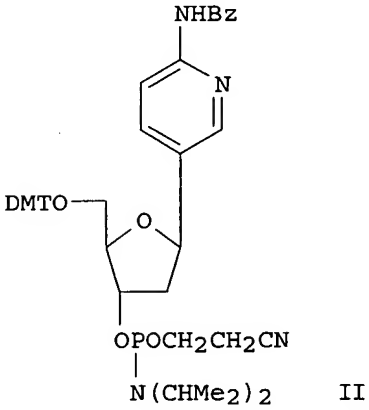

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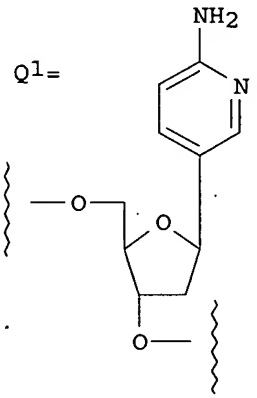

AB 5'-D(TTTTTXTXTXTXTXT) (X = Q1), prepared using phosphoramidite (I) (preparation given) showed a dramatic increase in Tm for third-strand dissociation from a 21-mer duplex. Due to enhanced basicity, Q1 is an excellent substitute for cytidine in DNA duplex recognition at physiol. pH through the py:pu-py motif. The lack of the 2-oxo function does not perturb third-strand binding in the major groove of DNA.

L27 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:322759 HCAPLUS
DOCUMENT NUMBER: 125:143183
TITLE: Synthesis of carbocyclic C-nucleosides containing non-natural pyrimidine bases

AUTHOR(S): **Hildbrand, Stefan**; Leumann, Christian; Scheffold, Rolf
CORPORATE SOURCE: Inst. organische Chemie, Univ. Bern, Bern, CH-3012, Switz.
SOURCE: Helvetica Chimica Acta (1996), 79(3), 702-709
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
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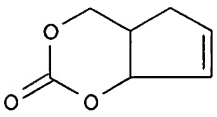

I

AB A series of carbocyclic C-nucleosides with a cis-4'-(hydroxymethyl)cyclopent-2'-enyl sugar moiety and unnatural pyrimidine bases were synthesized in racemic form in 2 steps starting from the easily accessible carbonate I.

L27 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:53074 HCAPLUS
DOCUMENT NUMBER: 122:10439
TITLE: A short synthesis of (-)-carbovir
AUTHOR(S): **Hildbrand, Stefan**; Troxler, Thomas; Scheffold, Rolf
CORPORATE SOURCE: Inst. Organ. Chem., Univ. Bern, Bern, CH-3012, Switz.
SOURCE: Helvetica Chimica Acta (1994), 77(5), 1236-40
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: English
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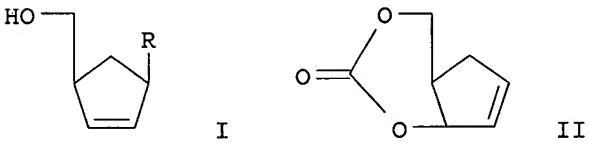

I II

AB Carbovir (-)-I (R = guanine) was synthesized via the cyclic carbonate II in four steps starting from enantiomerically enriched (cyclopentenyl)methanol (-)-I (R = H).

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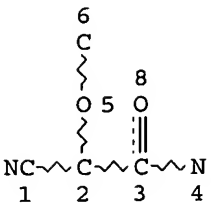
L1 STR



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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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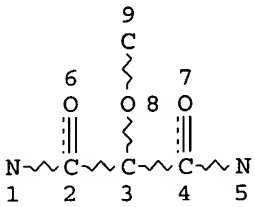
NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE
L3 31 SEA FILE=REGISTRY SSS FUL L1
L6 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
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GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
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L9 49 SEA FILE=REGISTRY ABB=ON PLU=ON TRIFLUOROACETIC ANHYDRIDE?/CN OR DIBUTYLTIN OXIDE?/CN OR PHOSPHORUS OXYCHLORIDE?/CN OR PHOSPHORUS TRICHLORIDE?/CN OR PHOSPHORUS PENTACHLORIDE?/CN
L11 643 SEA FILE=REGISTRY ABB=ON PLU=ON ALUMINUM CHLORIDE?/CN
L12 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L3
L13 70 SEA FILE=HCAPLUS ABB=ON PLU=ON L8
L14 25437 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 OR TRIFLUOROACETIC(W)ANHYDRIDE OR DIBUTYLTIN(W) OXIDE OR PHOSPHORUS(W)(OXYCHLORIDE? OR TRICHLORIDE OR PENTACHLORIDE?)
L15 73122 SEA FILE=HCAPLUS ABB=ON PLU=ON L11 OR ALUMINUM (W)CHLORIDE OR ALCL3
L16 389244 SEA FILE=HCAPLUS ABB=ON PLU=ON ("DEHYDRATION AGENTS"/CV OR "DEHYDRATION REACTION (L) AGENTS"/CV OR "DRYING AGENTS"/CV) OR DEHYDRAT? OR DRYING
L17 30094 SEA FILE=HCAPLUS ABB=ON PLU=ON ("LEWIS ACIDS"/CV OR "CARBONYLS (L) LEWIS ACID COMPLEXES"/CV OR "CHARGE TRANSFER COMPLEXES"/CV OR ELECTROPHILES/CV OR "LEWIS ACIDITY"/CV OR "LEWIS BASES"/CV) OR LEWIS(W)ACID
L20 4 SEA FILE=HCAPLUS ABB=ON PLU=ON (L8 AND (L16 OR L14 OR L17 OR L15)) NOT L12

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                 P"/AU) OR "BARTEK JOHANNES"/AU
L25          222 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("FUCHS R"/AU OR "FUCHS R
                 A"/AU OR "FUCHS R E M"/AU OR "FUCHS R F"/AU OR "FUCHS R J"/AU
                 OR "FUCHS R K"/AU OR "FUCHS R L"/AU OR "FUCHS R M"/AU OR
                 "FUCHS R P"/AU OR "FUCHS R P P"/AU OR "FUCHS R R"/AU OR "FUCHS
                 R WAYNE"/AU) OR "FUCHS RUDOLF"/AU
L26           15 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "HILDBRAND STEFAN"/AU
L27           14 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L26 NOT (L12 OR L20)
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                 (L12 OR L20 OR L27)


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L1                STR
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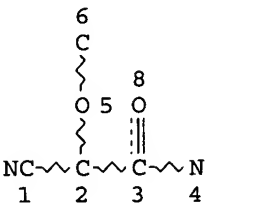


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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   7

STEREO ATTRIBUTES: NONE
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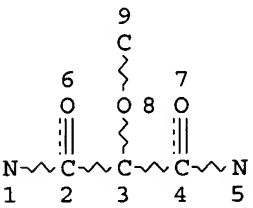


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS   9

STEREO ATTRIBUTES: NONE
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L9            49 SEA FILE=REGISTRY ABB=ON  PLU=ON  TRIFLUOROACETIC ANHYDRIDE?/CN
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                 PHOSPHORUS TRICHLORIDE?/CN OR PHOSPHORUS PENTACHLORIDE?/CN
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L12            8 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3
L14        25437 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L9 OR TRIFLUOROACETIC(W)ANHYDR
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                TRICHLORIDE OR PENTACHLORIDE?)
L15         73122 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11 OR ALUMINUM (W)CHLORIDE
                OR ALCL3
L16        389244 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("DEHYDRATION AGENTS"/CV OR
                "DEHYDRATION REACTION (L) AGENTS"/CV OR "DRYING AGENTS"/CV) OR
                DEHYDRAT? OR DRYING
L17         30094 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("LEWIS ACIDS"/CV OR "CARBONYL
                S (L) LEWIS ACID COMPLEXES"/CV OR "CHARGE TRANSFER COMPLEXES"/C
                V OR ELECTROPHILES/CV OR "LEWIS ACIDITY"/CV OR "LEWIS BASES"/CV
                ) OR LEWIS(W)ACID
L20             4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L8 AND (L16 OR L14 OR L17 OR
                L15)) NOT L12
L26            15 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "HILDBRAND STEFAN"/AU
L27            14 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L26 NOT (L12 OR L20)
L30          5603 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L16 OR L14) AND (L17 OR L15)

L31          1285 SEA FILE=REGISTRY ABB=ON  PLU=ON  MALONAMIDE?
L32          3721 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L31 OR ?MALOMAMIDE?
L33             8 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L32 AND L30
L34             7 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L33 NOT (L12 OR L20 OR L27)


=>
=>

=> d ibib abs hitstr l34 1-7

L34  ANSWER 1 OF 7  HCAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2005:203862  HCAPLUS
DOCUMENT NUMBER:          142:429941
TITLE:                    Process for preparation of malononitrile
INVENTOR(S):              Wu, Zongtao; Wang, Xinggen; Zhou, Jian; Wu, Kai
PATENT ASSIGNEE(S):       Peop. Rep. China
SOURCE:                   Faming Zhuanli Shenqing Gongkai Shuomingshu, 4 pp.
                          CODEN: CNXXEV
DOCUMENT TYPE:            Patent
LANGUAGE:                 Chinese
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     --------------       ----   --------    --------------------    --------
     CN 1451649            A     20031029    CN 2003-113472          20030512
PRIORITY APPLN. INFO.:                       CN 2003-113472          20030512
OTHER SOURCE(S):          CASREACT 142:429941
AB   This invention pertains to a method for producing malononitrile by
     dehydration of cyanoacetamide in 1,1,2-trichloroethane in the
     presence of AlCl3-diethylamine HCl- pyridine (1:1.2-1.8:0.5-1.5)
     composite catalyst and POCl3 dehydration agent at 50-114
     °C for 0.5-5 h under collecting product and absorbing HCl gas with
     adsorption tower.
IT   7446-70-0, Aluminum chloride, uses
     RL: CAT (Catalyst use); USES (Uses)
        (preparation of malononitrile by dehydration of cyanoacetamide)
RN   7446-70-0  HCAPLUS
CN   Aluminum chloride (AlCl3) (9CI)  (CA INDEX NAME)
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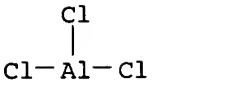
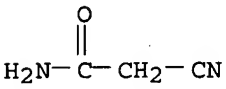
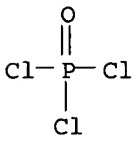


IT **107-91-5**, Cyanoacetamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of malononitrile by **dehydration** of cyanoacetamide)
RN 107-91-5 HCAPLUS
CN Acetamide, 2-cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **10025-87-3, Phosphorus oxychloride**
RL: RGT (Reagent); RACT (Reactant or reagent)
(preparation of malononitrile by **dehydration** of cyanoacetamide)
RN 10025-87-3 HCAPLUS
CN Phosphoric trichloride (9CI) (CA INDEX NAME)

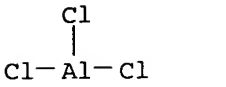


L34 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:220485 HCAPLUS
DOCUMENT NUMBER: 134:237219
TITLE: Process for preparing propanedinitrile
INVENTOR(S): Cao, Jianbing
PATENT ASSIGNEE(S): Zhennan Chemical Plant, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 8 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

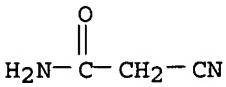
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1264701	A	20000830	CN 1999-100873	19990224

PRIORITY APPLN. INFO.: CN 1999-100873 19990224
OTHER SOURCE(S): CASREACT 134:237219
AB The process comprises aminating Me cyanoacetate with NH3 in methanol at (-5)-40°, **drying** at 50-110°, **dehydrating** with POCl3 in dichloroethane in the presence of catalyst at 40-90°, separating, and distilling at 130-135° and 1.8-2.2 kPa. The catalyst is composed of diethylamine HCl 1, anhydrous pyridine 1, and anhydrous **AlCl3** 1 part.
IT **7446-70-0, Aluminum chloride (AlCl3)**, uses
RL: CAT (Catalyst use); USES (Uses)

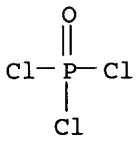
(process for preparing propanedinitrile)
RN 7446-70-0 HCAPLUS
CN Aluminum chloride (AlCl3) (9CI) (CA INDEX NAME)



IT **107-91-5P**, Cyanoacetamide
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for preparing propanedinitrile)
RN 107-91-5 HCAPLUS
CN Acetamide, 2-cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **10025-87-3, Phosphorus oxychloride**
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for preparing propanedinitrile)
RN 10025-87-3 HCAPLUS
CN Phosphoric trichloride (9CI) (CA INDEX NAME)



L34 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:862111 HCAPLUS
DOCUMENT NUMBER: 133:362558
TITLE: Process for preparing high-purity malononitrile
INVENTOR(S): Wu, Zongtao; Wang, Xinggen; Zhou, Jian
PATENT ASSIGNEE(S): Tongyuan Fine Chemical Plant, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 6 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

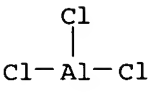
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1250773	A	20000419	CN 1998-111530	19981009
CN 1086691	B	20020626		

PRIORITY APPLN. INFO.: CN 1998-111530 19981009
OTHER SOURCE(S): CASREACT 133:362558
AB The process comprises reaction of Me cyanoacetate with NH3 at 10-60° to obtain cyanoacetamide, **dehydration** with POCl3 in organic solvent in the presence of catalyst at 60-90° for 4-12 h to

obtain crude malonitrile; recrystg. in anhydrous ethanol, and distilling at 109-120° and 16-22 mmHg. The catalyst is composed of diethylamine hydrochloride 1.2-1.8, **AlCl3** 1.0, and pyridine 0.5-1.5 part. The ratio of cyanoacetamide-POCl3-organic solvent-catalyst is 1:1.0-1.4:1.7-6.04:0.01-0.10. The organic solvent is methanol or ethanol.

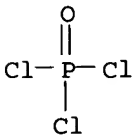
IT **7446-70-0**, Aluminum trichloride, uses
RL: CAT (Catalyst use); USES (Uses)
(preparation of high-purity malononitrile)

RN 7446-70-0 HCAPLUS
CN Aluminum chloride (AlCl3) (9CI) (CA INDEX NAME)



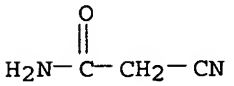
IT **10025-87-3**, Phosphoryl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of high-purity malononitrile)

RN 10025-87-3 HCAPLUS
CN Phosphoric trichloride (9CI) (CA INDEX NAME)



IT **107-91-5P**, Cyanoacetamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of high-purity malononitrile)

RN 107-91-5 HCAPLUS
CN Acetamide, 2-cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)



L34 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:716299 HCAPLUS
DOCUMENT NUMBER: 125:328111
TITLE: Process and phosphorous-compound catalysts for the preparation of nitriles from carboxamides
INVENTOR(S): Hermeling, Dieter; Siegel, Hardo
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 4 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

DE 19515989	A1	19961107	DE 1995-19515989	19950502
PRIORITY APPLN. INFO.:			DE 1995-19515989	19950502

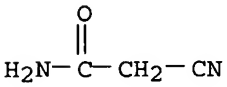
OTHER SOURCE(S): CASREACT 125:328111; MARPAT 125:328111

AB Nitriles R1CN [R1 = (un)substituted alkyl, (un)substituted cycloalkyl, (un)substituted Ph] (e.g., 1,8-dicyanooctane) are prepared in high yield and purity by the **dehydration** of carboxamides R1CONH2 (e.g., decanedicarboxylic acid diamide) at 20-150°/0.01-5 bar in a suspension in an inert solvent (e.g., PhMe) in the presence of a P compound catalyst (e.g., Ph3P:O) or their adducts with acids (e.g., phosgene) or **Lewis acids.**

IT **107-91-5**, Cyanoacetamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(process and phosphorous-compound catalysts for the preparation of nitriles from carboxamides)

RN 107-91-5 HCAPLUS

CN Acetamide, 2-cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)



L34 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1978:546397 HCAPLUS

DOCUMENT NUMBER: 89:146397

TITLE: Studies on the optimization of cyanoacetamide to malononitrile **dehydration**

AUTHOR(S): Malinowski, Romuald; Legocki, Jan

CORPORATE SOURCE: Pol.

SOURCE: Organika (1977) 53-61
CODEN: ORGAD2; ISSN: 0137-9933

DOCUMENT TYPE: Journal

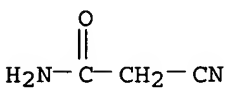
LANGUAGE: Polish

AB The **dehydration** of cyanoacetamide to CH2(CN)2 with POCl3 in the presence of small amts. of CaCl2 or **AlCl3**, to prevent formation of polymeric metaphosphoric acid, was studied. Thus, cyanoacetamide (1 mol) and 0.12 mol CaCl2 or 0.05 mol **AlCl3** are added to 168-210 g EtCl. The mixture is stirred and then 0.7 mol POCl3 is gradually added. The reaction mixture is heated to 90° for 6-7 h, then cooled to 20°. The filtrate is distilled at 10-15 mm Hg to give a yield of 88.4%.

IT **107-91-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**dehydration** of)

RN 107-91-5 HCAPLUS

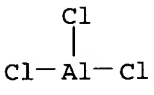
CN Acetamide, 2-cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **7446-70-0**, uses and miscellaneous
RL: USES (Uses)
(**dehydration** of cyanoacetamide in presence of)

RN 7446-70-0 HCAPLUS

CN Aluminum chloride (AlCl3) (9CI) (CA INDEX NAME)



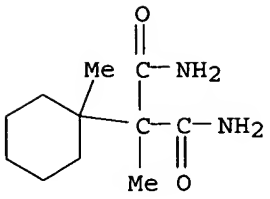
L34 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1958:11281 HCAPLUS
DOCUMENT NUMBER: 52:11281
ORIGINAL REFERENCE NO.: 52:2062c-f
TITLE: Substituted methylmalononitriles
INVENTOR(S): Westfahl, Jerome C.
PATENT ASSIGNEE(S): B. F. Goodrich Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2802019		19570806	US	

AB Derivs. of methylmalononitrile were prepared by the addition of aliphatic and alicyclic hydrocarbons possessing a tertiary C atom to 1,1-dicyanoethene (I). To a mixture of 133.3 parts anhydrous sublimed **AlCl3** and 250 ml. dry (Cl2CH)2 (II) was added in 47 min. with stirring at 40° a solution of I 41.5, isopentane (dried with P2O5) 36.1 parts, and 150 ml. II. The mixture was stirred 30 min. without heating and then hydrolyzed by pouring into 1 l. crushed ice containing 50 ml. concentrated HCl. The usual processing gave 2,2-dicyano-3,3-dimethylpentane, m. 44.4° (MeOH). Similarly was prepared 1-(1-methylcyclohexyl)-1-methylmalononitrile (III), b. 99-9.5°. Hydrolysis of 4.9 parts III with 20 ml. 95% H2SO4 at 90° for 5 min., pouring into 200 ml. cold H2O and washing the precipitate with 5% NaOH, and then H2O followed by **drying** gave 1-(1-methylcyclohexyl)-1-methylcyanoacetamide, m. 154.3-55° (C6H6-C6H14). III 10 and KOH 30 parts in H2O 30 and EtOH 125 ml. were refluxed 263 hrs. More H2O was then added and the EtOH distilled Acidification of the distillant to Congo red, shaking with Et2O and filtration gave (1-methylcyclohexyl)methylmalonamide, m. 239° (EtOH). The above H2O and Et2O layers were separated and the aqueous layer extracted with Et2O. This extract was combined with the Et2O layer and extracted with aqueous NaHCO3. The resulting H2O layer was separated and acidified to give (1-methylcyclohexyl)methylcyanoacetic acid (IV), m. 103.5-4.5° (C6H6-C6H14). Heating IV gave 1-(1-methylcyclohexyl)propionitrile (V), b. 220-7°, n25D 1.4631. Heating V with 95% H2SO4 gave 1-(1-methylcyclohexyl)propionamide, m. 108-8.5° (C6H6-C6H14) .

IT **99991-57-8**, Cyclohexanemalonamide, α,1-dimethyl-
(preparation of)

RN 99991-57-8 HCAPLUS
CN Cyclohexanemalonamide, α,1-dimethyl- (6CI) (CA INDEX NAME)



L34 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1949:11226 HCAPLUS
DOCUMENT NUMBER: 43:11226
ORIGINAL REFERENCE NO.: 43:2271e-i,2272a-i,2273a-i,2274a-b
TITLE: Biosynthesis of penicillins. III. Preparation and evaluation of precursors for new penicillins
AUTHOR(S): Behrens, Otto K.; Corse, Joseph; Huff, Dorothea E.; Jones, Reuben G.; Soper, Quentin F.; Whitehead, Calvert W.
SOURCE: Journal of Biological Chemistry (1948), 175, 771-92
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Methods are described for evaluation of compds. as precursors for new penicillins: (a) The ratio of units in the test container to units in control. Comparable results were obtained from P. notatum NRRL 1976 and P. chrysogenum Q-176. Stimulation may be interpreted as utilization of compound as a precursor. Lack of stimulation does not necessarily mean lack of utilization. (b) The ratio of antibacterial activity for Bacillus subtilis to that for Staphylococcus aureus compared with the same ratio using pure benzylpenicillin, which is defined as 1.0. (c) The relative position of the active portion in an adsorption column indicates a new penicillin. Culturing with N-2-hydroxyethyl-α-(allylmercapto)acetamide (I) deposited a new penicillin in a column. (d) The Craig method was used to determine the distribution coeffs. of the penicillins (C.A. 41, 6672i) formed between acid and ether. The penicillin formed using p-HSC6H4SCH2CO2H showed coeffs. and activities different from the controls while the activities and coeffs. with p-H2O3AsC6H4NHSO2C6H4SCH2CO2H-p as test precursor were similar to the controls. (e) Attempts were made to isolate the penicillin. With N-allyl-β-chloropropionamide as precursor the active material was recovered as the Na salt, 900 units/mg., distribution coefficient 0.64, but Cl in the product was below theory. β,β-Diphenylpropionic acid led to a penicillin, 1700 units/mg., coefficient 0.84, containing no diphenylpropionic group, but probably an aliphatic acyl group (UV absorption). Tryparsamide led to no As in the recovered penicillin; similarly, 2-thiophenecarboxylic acid and some derivs. were not utilized. Data obtained by these methods are presented for many compds. including aryl carboxylic acids, α-substituted phenylacetic acids, aliphatic acids, aryl aliphatic (other than acetic) acids, a miscellaneous unclassified group of acids, and derivs. of these acids. Preparation and some properties of new compds. in the above series are presented. Methods of preparation were: (A) The Schotten-Baumann method was applied to the acid chloride and the amino compound, allylamine, HOCH2CH2NH2, or DL-valine. (B) The Et or Me ester was heated with the amine. (C) EtSH (40 g.) was allowed to react with CH2:CHCO2Me (43 g.) in the presence of Triton B (2 drops) to form EtSCH2CH2CO2Me (61 g.), b55 109-13°. (D) CH2:CHCH2SCH2CONHCH2CH2OH (Soper, et al. J. Am. Chemical Society 70, 2849-55(1948)) (53.0 g.) in 100 mL. Me2CO was treated with 33.0

mL. 30% H2O2 for 1 wk. N-2-hydroxyethyl-α-(allylsulfinyl)acetamide (II) was recrystd. from EtOAc or EtOAc-MeOH. (E) CH2:CHCH2SCH2CONHCH2CH2OH (44.5 g.) in 1 l. Me2CO with 75 mL. 30% H2O2 was allowed to stand 10 days yielding 47.4 g. of the sulfonyl compound (III), an orange oil. (F) Addition of CH2:CHCOOMe (100 g.) to 200 mL. CH2:CHCH2OH, in which was dissolved 5.3 g. Na, produced a gelatinous precipitate The mixture was heated 1 h., poured into water, and extracted with ether. The ether solution was dried and distilled, b65 116-32°, n20.5D, 1.4312, yield 50.3 g., mainly Me β-(allyloxy)propionate. The 2nd fraction b65 120-30°, n20.5D 1.4394, yield 23.5 g., was chiefly the allyl ester. (G) DL-Alanyl-DL-valine (Fischer and Scheibler, C.A. 3, 315) was treated with p-ClC6H4COCl and NaOH to give about 90% N-[N-(p-chlorobenzoyl)-DL-alanyl]-DL-valine (IV), m. 204-6° (from dilute EtOH). p-ClC6H4CO2H contaminant was removed by washing with ether. (H) CH.tplbond.CCMe2OH (Hurd and McPhee, C.A. 41, 4095g) (130 g.), CuO (10 g.), NH4Cl (5 g.) and concentrated HCl (225 mL.) were shaken together 0.5 h. below 40°, and the non-aqueous layer washed with HCl, dried, and fractionated to yield 34% CH.tplbond.CCMe2Cl, b. 77-9° (Favorskii and Favorskaya, C.A. 39, 3651.4). This compound (194 g.) was treated with malonic ester (330 g.) in 1 l. absolute alc. in which had been dissolved 46 g. Na, the mixture filtered, the alc. evaporated under vacuum, the residual sirup treated with dilute cold HCl, extracted with ether, the ether solution washed and dried, the ether evaporated, and the remaining liquid fractionated in vacuo through a Vigreux column to give 192 g. (45%) CH.tplbond.CCMe2CH(CO2Et)2, b3 102-4°; from this was derived 148 g. (98%) of the crystalline acid, m. 105-6°. The acid was decarboxylated by heating at 180-200° 1-2 h. to 85% CH.tplbond.CCMe2CH2CO2H (IVa), b2 75-7° (bath temperature 130°); Me ester b. 150-3°, 65% yield. (I) Chloroacetylvaline (9.4 g.) was added to 10 g. PhAsCl2 in 30 mL. 10 N NaOH (Quick and Adams, C.A. 16, 1560). After dilution, filtering, and acidification, an oil precipitated which on recrystn. from water gave 8.5 g. CHMe2CH(COOH)NHCOCH2.As(O2H)Ph (V), m. 188° (decomposition). (J) To the Grignard reagent from m-(CF3)C6H4Br, Mg, and dry ether 0.15 g. powdered Se was added (Morgan and Porritt, C.A. 19, 3260) and the mixture hydrolyzed. After the ether layer was separated, washed, and extracted with 3 N NaOH, the resulting aqueous extract was added to 0.15 mol ClCH2CO2Na in 100 mL. water. In a few min. the mixture was acidified. Alternate extns. with ether and alkaline solution and acidification gave m-(CF3)C6H4SeCH2CO2H (Va) b7 140-2°, m. 58.5-9.5°. (K) Cl(CH2)3CN (52 g.), PhSH (56 g.), and NaOMe (28 g.) in 300 mL. absolute alc. was refluxed with stirring overnight. After the solvent was evaporated, the organic layer was washed and distilled in vacuo to give 72 g. impure PhS(CH2)3CN b0.1 135-7°; the acid obtained on hydrolysis m. 58-60°. (L) Br(CH2)4CO2Et, PhSH, and NaOEt in absolute alc. produced PhS(CH2)4CO2Et, b0.2 121-4°. (M) HO2C(CH2)4CO2Et (87 g.) with SOCl2 formed the chloride, which with PhCl, **AlCl3**, and CS2 gave 66.4 g. p-ClC6H4CO(CH2)4CO2Et, m. 59-60°; saponification with KOH gave the acid, m. 134-6°. Reduction with Zn and HCl in toluene-water, followed by treatment with MeOH resulted in p-ClC6H4(CH2)5CO2Me, b0.4 122-5°. (N) (p-ClC6H4)2CO was converted by the Reformatskii reaction to 90% (p-ClC6H4)2C(OH)CH2CO2Et, m. 96-7°, **dehydrated** by P2O5 in C6H6 and saponified to (p-ClC6H4)2C:CHCO2H, m. 173-4°. The acid was allowed to take up 0.10 mol H at 4 atmospheric over 5% Pd on C to yield 71% (p-ClC6H4)2CHCH2CO2H (VI), m. 182-3°. (O) Desoxyanisoin and BrCH2CO2Et in dry C6H6 was treated with Zn dust, the reaction mixture shaken

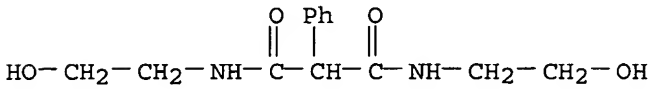
with dilute H2SO4, the C6H6 layer separated and dried, and, after removal of the C6H6, the product distilled in vacuo with **dehydration** to 90% Et β,γ-bis(p-methoxyphenyl)butenoate, b2 221°; hydrogenation and saponification gave 90% β,γ-bis(p-methoxyphenyl)butyric acid (VII), m. 167-8°. Data on precursors are given in the order: acid, N-substituted amide, method of preparation (or taken from the literature or purchased com.), m.p. or b.p. of amide, stimulation (see Test a) of the amide (if no amide is given, value is for the acid): NCCH2CO2H, HOCH2CH2, B, oil, 0.9; ClCH2CH2CO2H, allyl, A, 39-40°, 1.0; HOCH2CH2CO2H, HOCH2CH2, B, 73.5-75, 1.0; γ,γ,γ-trichlorobutyric, DL-valine, A, 197, 1.0; CF3CH(OH)CH2CO2H, HOCH2CH2, B, 59-61, 1.1; CH2:CHCH2CO2H, HOCH2CH2, A, b1 138-42, 1.4; (ethylmercurimercapto)acetic, -, -, -, toxic; β-hydroxybutyric, HOCH2CH2, B, 68-71, 1.0; MeOCH2CH2CO2H, HOCH2CH2, B, b1.5 142-5, 1.0; 2-thiophenecarboxylic (VIII), HOCH2CH2, B, 90-1, 1.0; VIII, allyl, A, 65, 1.0; VIII, DL-valine, A, 123-4, 1.0; allylsulfinylacetic, II, D, 81.5-82, 1.2; allylsulfonylacetic, III, E, oil, 0.9; EtSCH2CH2CO2H (C), HOCH2CH2, B, b0.45 173-5, 1.0; sorbic, HOCH2CH2, B, b1 158-60, 1.1; β-allyloxypropionic (F), HOCH2CH2, B, b0.3 142-4, 0.8; tert-butylacetic, DL-valine, A, 147-8, 0.8; isocaproic, DL-valine, A, 100-1, 1.0; γ-ethoxybutyric, HOCH2CH2, B, b1 138-40, 1.0; p-ClC6H4CO2H (IX), HOCH2CH2, A, 113-14, 1.0 (acid alone, 1.0); IX, allyl, A, 73, 1.0; IX, DL-valine, A, 178-9, 1.0; IX, DL-alanyl-DL-valine, G, 204-6, 1.0; BzOH (X), allyl, -, -, 0.9; X, 2-benzamido-1,3-propanediol, B, 67-9, 1.0; p-O:AsC6H4CH2CO2H, -, -, -, 1.0; PhCH2SO2H, DL-valine, A, 120-3, 1.0; IVa, (H), HOCH2CH2, B, b0.5 150-5, 0.8; cyclopentylacetic, HOCH2CH2, B, 57-8, 1.6; hexahydrobenzoic, DL-valine, A, 195-7, 1.0; BzCO2H, -, -, -, 1.0; mandelic, HOCH2CH2, B, 61-4, 1.0; PhSeCH2CO2H, HOCH2CH2, A, 56-8, 1.2 (acid alone, 1.8); PhSO2CH2CO2H, HOCH2CH2, B, 93-4, 1.1 (acid alone, 1.0); Ph(HO2)AsCH2CO2H, DL-valine, I, 188 (dec.), 1.0 (acid alone, toxic); C6H11CH2CO2H (XI), HOCH2CH2, B, 66-8, 1.0; XI, DL-valine, A, 178-9, 1.1; δ-carbethoxyvaleric, HOCH2CH2, A, oil, 1.0; PhC.tplbond.CCO2H, -, -, -, 0.9; NCCHPhCO2H, HOCH2CH2, B, 105-7, 0.8; Va, -, J, 58.5-9.5, 1.0; cinnamic (XII), HOCH2CH2, B, 101, 1.0; XII, DL-valine, A, 183-4, 1.0; XII, allyl, A, 90-2, 0.9; (2,4-dichlorobenzylsulfonyl)acetic, -, -, -, 0.9; PhCH(CO2H)2, bis(2-hydroxyethyl), B, oil, 1.2; (p-chlorobenzylsulfonyl)acetic, -, -, -, 0.9; hydrocinnamic, DL-valine, A, 141-3, 1.0; MeCH(SPh)CO2H, -, -, -, 1.3; PhSCH2CH2CO2H, DL-valine, A, 93-4, 1.1; MeOCHPhCO2H, HOCH2CH2, B, 84-7, 1.0; tropic, HOCH2CH2, B, oil, 1.2; PhCH2SO2CO2H, -, -, -, 1.0; N-phenylsarcosine, HOCH2CH2, B, 56-7, 1.0; (p-chlorocarbobenzoxy)glycine, -, -, 108-9.5, 1.0; γ-(2,4-dichlorophenoxy)butyric, -, -, -, toxic; styrylacetic, allyl, A, 61-3, 1.4; β-(p-bromophenyl)butyric, DL-valine, A, 134-5, 2.5; carbobenzoxyglycine, -, -, -, 1.2; γ-(p-nitrophenyl)butyric, DL-valine, A, 138-43, 1.5; EtCHPhCO2H, DL-valine, A, oil, 1.0; Me2CPhCO2H, DL-valine, A, oil, 1.1; β-phenylbutyric, HOCH2CH2, B, oil, 0.9; γ-phenylmercaptobutyric, -, K, 58-60, 2.0; γ-phenoxybutyric, HOCH2CH2, B, 70-2, 1.0; γ-(p-aminophenyl)butyric, DL-valine, obtained by catalytic hydrogenation of the nitro compound, 175-9, 0.8; fencholic, -, -, -, toxic; γ-cyclohexylbutyric, HOCH2CH2, B, 45-8, 1.1; capric, HOCH2CH2, -, 75, 1.0; 3-indolepropionic, -, -, -, 0.9; γ-benzoylbutyric, -, -, -, 1.0; benzylsuccinic, -, -, -, 1.0; γ-(p-bromophenyl)isovaleric, DL-valine, A, 109-10, 0.8; β-(p-chlorophenyl)isovaleric, -, -, -, 0.5; β-(p-fluorophenyl)isovaleric, -, -, -, 0.9; β-(p-iodophenyl)isovaleric, -, -, -, toxic; β-(p-nitrophenyl)isovaleric, DL-valine, A, 110-15, 1.3; δ-phenylvaleric, DL-valine, A, 98-100, 0.8; δ-phenylmercaptovaleric (L), HOCH2CH2, B, 91-2, 1.0; β-(p-

hydroxyphenyl)isovaleric, -, -, -, 1.0; β-(p-aminophenyl)isovaleric, -, -, -, 1.0; p-Me3SiC6H4SeCH2CO2H, -, -, b4 170-3, toxic; cyclohexylvaleric, -, -, -, toxic; 10-hendecenoic, HOCH2CH2, B, 66-7, 1.0; 3-indolebutyric, HOCH2CH2, B, oil, 1.0; ε-(p-chlorophenyl)caproic (M), HOCH2CH2, B, oil, 1.4; lauric, HOCH2CH2, B, 86-7, 0.9; 1-naphthalenepropionic, HOCH2CH2, B, 60-1, 1.0; 6-benzoyl-3-ketocaproic, -, -, -, 1.0; γ-mesitylbutyric, -, -, 82-4, toxic (acid); Ph2CHCO2H, HOCH2CH2, B, 118-19, 1.0; myristic, HOCH2CH2, B, 94-5, 1.0; VI (N), DL-valine, A, 155-6, 0.9 (acid alone 0.4); Ph2CHCH2CO2H, HOCH2CH2, B, 94, 0.9; 4-methoxy-1-naphthalenebutyric, HOCH2CH2, B, oil, 0.6; (PhCH2)2CHCO2H, HOCH2CH2, B, 83-4, 0.9; palmitic, HOCH2CH2, B, 97.5, 1.0; β,β-di-p-tolylpropionic, HOCH2CH2, B, 85-6, 0.9; 9-(p-iodophenyl)hendecanoic, HOCH2CH2, B, oil, 1.0; 3-phenylhendecanoic, HOCH2CH2, B, oil, 1.0; linoleic, HOCH2CH2, B, b1 215-20, 0.9; VII (O), DL-valine, A, 147-8, 1.0; ricinoleic, HOCH2CH2, B, 54-5, 1.0; 9,10-dihydroxystearic, HOCH2CH2, B, 150, 1.4; β-1-pyrenoylpropionic (C20H14O3), -, -, -, toxic.

IT **860374-08-9**, Malonamide, N,N'-bis(2-hydroxyethyl)-2-phenyl-
(in penicillin production)

RN 860374-08-9 HCAPLUS

CN Malonamide, N,N'-bis(2-hydroxyethyl)-2-phenyl- (5CI) (CA INDEX NAME)



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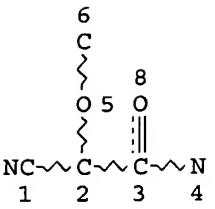

NODE ATTRIBUTES:
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L36 2 SEA FILE=CASREACT SSS FUL L1 (35 REACTIONS)

100.0% DONE 802 VERIFIED 35 HIT RXNS 2 DOCS
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L36 ANSWER 1 OF 2 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 142:23494 CASREACT
TITLE: Three-Component Condensation Leading to β-Amino Acid Diamides: Convergent Assembly of β-Peptide Analogues
AUTHOR(S): Oaksmith, Jennifer M.; Peters, Ulf; Ganem, Bruce
CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Baker Laboratory, Cornell University, Ithaca, NY, 14853-1301, USA
SOURCE: Journal of the American Chemical Society (2004), 126(42), 13606-13607
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A Passerini condensation of acyl cyanides, carboxylic acids, and isonitriles has been developed that affords efficient access to functionalized diamides as well as β-peptides of α-hydroxy-β-amino acids. Such compds. are protease-resistant and form stable helical and sheet structures when incorporated into larger peptides (no data given). N-Protected α-amino acids and isocyanoesters derived from α-amino acids participate in the condensation, leading to α/β peptides embodying the heterogeneous α/β/α backbone motif.

RX(1) OF 45 A + B + C ===> D...

RX(1) RCT A 631-57-2, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT C 931-53-3
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO D **799778-66-8**
NTE no solvent, Passerini condensation

RX(2) OF 45 E + B + C ===> **F**...

RX(2) RCT E 58040-74-7, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT C 931-53-3
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO F **799778-69-1**
NTE no solvent, Passerini condensation

RX(3) OF 45 G + B + C ===> **H**

RX(3) RCT G 68077-52-1, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT C 931-53-3
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO H **799778-72-6**
NTE no solvent, Passerini condensation

RX(4) OF 45 I + B + C ===> **J**

RX(4) RCT I 42867-40-3, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT C 931-53-3
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO J **799778-75-9**

NTE no solvent, Passerini condensation

RX(5) OF 45 K + B + C ===> **L**

RX(5) RCT K 799779-56-9, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT C 931-53-3
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO L **799778-78-2**
NTE no solvent, Passerini condensation

RX(6) OF 45 A + M + C ===> **N**

RX(6) RCT A 631-57-2, M 124-07-2

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT C 931-53-3
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO N **799778-83-9**
NTE no solvent, Passerini condensation

RX(7) OF 45 E + M + C ===> **O...**

RX(7) RCT E 58040-74-7, M 124-07-2

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT C 931-53-3
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO O **799778-85-1**
NTE no solvent, Passerini condensation

RX(8) OF 45 A + B + P ===> **Q...**

RX(8) RCT A 631-57-2, B 64-19-7

STAGE(1)

CON 10 minutes, 0 deg C

STAGE(2)
RCT P 7188-38-7
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO Q **799778-93-1**
NTE no solvent, Passerini condensation

RX(9) OF 45 E + B + P ===> **R**

RX(9) RCT E 58040-74-7, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT P 7188-38-7
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO R **799778-98-6**
NTE no solvent, Passerini condensation

RX(10) OF 45 A + B + S ===> **T**

RX(10) RCT A 631-57-2, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT S 2769-64-4
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO T **799779-07-0**
NTE no solvent, Passerini condensation

RX(11) OF 45 A + B + U ===> **V**

RX(11) RCT A 631-57-2, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT U 2999-46-4
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO V **799779-11-6**
NTE no solvent, Passerini condensation

RX(12) OF 45 A + B + W ===> **X...**

RX(12) RCT A 631-57-2, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT W 43219-50-7
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO X **799779-16-1**
NTE no solvent, Passerini condensation

RX(13) OF 45 I + M + W ===> **Y**

RX(13) RCT I 42867-40-3, M 124-07-2

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT W 43219-50-7
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO Y **799779-19-4**
NTE no solvent, Passerini condensation

RX(14) OF 45 A + B + Z ===> **AA...**

RX(14) RCT A 631-57-2, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT Z 799779-64-9
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO AA **799779-25-2**
NTE no solvent, Passerini condensation

RX(15) OF 45 A + B + AB ===> **AC**

RX(15) RCT A 631-57-2, B 64-19-7

STAGE(1)
CON 10 minutes, 0 deg C

STAGE(2)
RCT AB 799779-66-1
CON SUBSTAGE(1) 0 deg C -> room temperature
SUBSTAGE(2) 1 hour, room temperature

PRO AC **799779-28-5**
NTE no solvent, Passerini condensation

RX(16) OF 45 A + AD + C ===> **AE**

RX(16) RCT A 631-57-2, AD 140-10-3, C 931-53-3
PRO AE **799778-81-7**
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 12 hours, room temperature
NTE Passerini condensation

RX(17) OF 45 G + AG + C ===> **AH**

RX(17) RCT G 68077-52-1, AG 501-52-0, C 931-53-3
PRO AH **799778-88-4**
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 12 hours, room temperature
NTE Passerini condensation

RX(18) OF 45 E + AI + C ===> **AJ**

RX(18) RCT E 58040-74-7, AI 65-85-0, C 931-53-3
PRO AJ **799778-90-8**
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 12 hours, room temperature
NTE Passerini condensation

RX(19) OF 45 A + AK + P ===> **AL**

RX(19) RCT A 631-57-2, AK 1161-13-3, P 7188-38-7
PRO AL **799779-01-4**
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 12 hours, room temperature
NTE Passerini condensation

RX(20) OF 45 A + AM + P ===> **AN...**

RX(20) RCT A 631-57-2, AM 13734-34-4, P 7188-38-7
PRO AN **799779-04-7**
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 12 hours, room temperature
NTE Passerini condensation

RX(21) OF 45 K + AI + S ===> **AO...**

RX(21) RCT K 799779-56-9, AI 65-85-0, S 2769-64-4
PRO AO **799779-09-2**
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 12 hours, room temperature
NTE Passerini condensation

RX(22) OF 45 K + AG + U ===> **AP...**

RX(22) RCT K 799779-56-9, AG 501-52-0, U 2999-46-4
PRO AP **799779-13-8**
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 12 hours, room temperature
NTE Passerini condensation

RX(23) OF 45 A + AK + Z ===> **AQ**

RX(23) RCT A 631-57-2, AK 1161-13-3, Z 799779-64-9
PRO AQ **799779-22-9**
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 12 hours, room temperature
NTE Passerini condensation

RX(24) OF 45 A + AM + Z ===> **AR...**

RX(24) RCT A 631-57-2, AM 13734-34-4, Z 799779-64-9
PRO AR **799779-30-9**
SOL 75-09-2 CH2Cl2
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 12 hours, room temperature
NTE Passerini condensation

RX(25) OF 45 **...D** ===> AS

RX(25) RCT D **799778-66-8**

STAGE(1)
RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 22 hours, room temperature

STAGE(2)
RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)
RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO AS 799779-32-1
NTE stage 1 chemoselective

RX(26) OF 45 ...2 **F** + AX ===> AY + AZ

RX(26) RCT F **799778-69-1**, AX 67-56-1

STAGE(1)
RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 46 hours, room temperature

STAGE(2)
RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)
RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO AY 799779-35-4, AZ 851165-95-2
NTE stage 1 chemoselective

RX(27) OF 45 ...**O** ===> BA

RX(27) RCT O **799778-85-1**

STAGE(1)
RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 46 hours, room temperature

STAGE(2)
RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)
RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO BA 799779-37-6
NTE stage 1 chemoselective

RX(28) OF 45 ...**Q** ===> BB

RX(28) RCT Q **799778-93-1**

STAGE(1)
RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 23 hours, room temperature

STAGE(2)
RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)
RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO BB 799779-39-8
NTE stage 1 chemoselective, alternate one-pot two-step synthesis shown

RX(29) OF 45 ...**AO** ===> BC

RX(29) RCT AO **799779-09-2**

STAGE(1)
RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 46 hours, room temperature

STAGE(2)
RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)
RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO BC 799779-43-4
NTE stage 1 chemoselective

RX(30) OF 45 ...2 **AP** + 2 AX ===> BD + BE

RX(30) RCT AP **799779-13-8**, AX 67-56-1

STAGE(1)
RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 22 hours, room temperature

STAGE(2)
RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)
RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO BD 799779-45-6, BE 851166-00-2
NTE stage 1 chemoselective

RX(31) OF 45 ...**X** ===> BF

RX(31) RCT X **799779-16-1**

STAGE(1)
RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 23 hours, room temperature

STAGE(2)
RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)
RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO BF 799779-47-8
NTE stage 1 chemoselective

RX(32) OF 45 ...**AA** ===> BG

RX(32) RCT AA **799779-25-2**

STAGE(1)
RGT AT 7647-01-0 HCl, AU 1333-74-0 H2
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 16 hours, room temperature

STAGE(2)
RGT AV 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature, pH 8
SUBSTAGE(2) 10 minutes, room temperature, pH 8

STAGE(3)
RGT AT 7647-01-0 HCl
SOL 67-56-1 MeOH
CON room temperature, pH 6

PRO BG 799779-49-0
NTE stage 1 chemoselective

RX(33) OF 45 ...**AN** ===> BH

RX(33) RCT AN **799779-04-7**
RGT AU 1333-74-0 H2
PRO BH 799779-41-2
CAT 7440-05-3 Pd
SOL 109-99-9 THF
CON 16 hours, room temperature
NTE chemoselective, product depends on solvent

RX(34) OF 45 ...**AR** ===> BJ

RX(34) RCT AR **799779-30-9**
RGT AU 1333-74-0 H2
PRO BJ 799779-50-3
CAT 7440-05-3 Pd, 7440-02-0 Ni
SOL 109-99-9 THF
CON 25 hours, room temperature
NTE chemoselective, product depends on solvent, Raney nickel used
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 2 OF 2 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 135:152562 CASREACT
TITLE: Dehydration method for producing 2-(alkoxy)malonodinitriles from 2-alkoxymalondiamides
INVENTOR(S): Bartek, Johannes; Fuchs, Rudolf; Hildbrand, Stefan
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 13 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001058857	A1	20010816	WO 2001-EP1505	20010209
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, US, US, US, US				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001033759	A5	20010820	AU 2001-33759	20010209
EP 1254105	A1	20021106	EP 2001-905765	20010209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003522753	T2	20030729	JP 2001-558409	20010209
US 2003144538	A1	20030731	US 2002-182716	20021011
US 6673957	B2	20040106		
US 2004063987	A1	20040401	US 2003-673988	20030930

PRIORITY APPLN. INFO.:
EP 2000-102758 20000210
EP 2000-109505 20000504
US 2001-267087P 20010207
WO 2001-EP1505 20010209
US 2002-182716 20021011

OTHER SOURCE(S): MARPAT 135:152562

AB 2-(Alkoxy)malonodinitriles (NC)2CHOR (R = C1-6 alkyl, halogen-substituted C1-6 alkyl) (e.g., 2-methoxymalonodinitrile) or 2-(alkoxy)-2-cyanoacetamides are prepared by the dehydration of the corresponding 2-alkoxymalondiamides (H2NCO)2CHOR in the presence of a dehydrating agent (e.g., POCl3).

RX(2) OF 2 A ===> **F**

RX(2) RCT A 5018-31-5
RGT C 10025-87-3 POCl3
PRO F **353291-71-1**
CAT 7446-70-0 AlCl3
SOL 75-05-8 MeCN

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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